Jan Deboral please

Access DB# 110639

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Sabiha Qazi Examiner #: 74141 Date: 12/16/03
Art Unit: 1646 Phone Number 305-3910 Serial Number: 09/939,208
Mail Box and Bldg/Room Location: 2D19 Results Format Preferred (circle): ~~PAPER~~ DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Angiogenic agent See 09/479,331

Inventors (please provide full names): Gregory E. Agoston et al

Earliest Priority Filing Date: 2/8/2001

***For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.**

Please search for elected species of Cl. 3, (Structure attached) and compds of formula in Cl 1

****

STAFF USE ONLY	Type of Search		Vendors and cost where applicable	
Searcher: Jan 4496	NA Sequence (#)		STN	V
Searcher Phone #:	AA Sequence (#)		Dialog	
Searcher Location:	Structure (#)	V	Questel/Orbit	
Date Searcher Picked Up: 12/21	Bibliographic		Dr.Link	
Date Completed: 12/21	Litigation		Lexis/Nexis	
Searcher Prep & Review Time:	Fulltext		Sequence Systems	
Clerical Prep Time: 20	Patent Family		WWW/Internet	
Online Time: 75	Other		Other (specify)	

PTO-1590 (8-01)

Sabina:
Claim 1b, page 2, contains (an) error:

$CH_2-C\equiv R \rightarrow CH_2-C\equiv H$!

Also, I had to leave R_a, R_{h1}, R_{h2}, R_g, R_5, and R_{g2} open, as they are "optionally" substituted ....!

Broader, from applicants' own references

Elected Species

=> fil reg
FILE 'REGISTRY' ENTERED AT 09:14:10 ON 21 DEC 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 19 DEC 2003 HIGHEST RN 628722-21-4
DICTIONARY FILE UPDATES: 19 DEC 2003 HIGHEST RN 628722-21-4

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

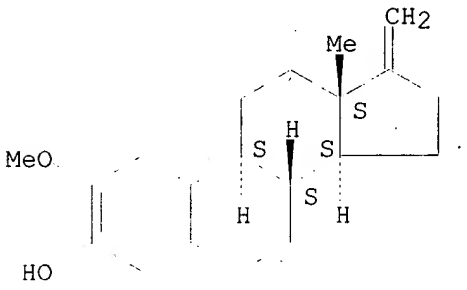
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> d l3 ide can

L3 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS on STN
RN 431901-73-4 REGISTRY
CN **Estra-1,3,5(10)-trien-3-ol, 2-methoxy-17-methylene- (9CI)** (CA INDEX NAME)
FS STEREOSEARCH
MF **C20 H26 O2**
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:47357

REFERENCE 2: 137:6309

=> fil uspatall
FILE 'USPATFULL' ENTERED AT 09:14:17 ON 21 DEC 2003

FILE 'USPAT2' ENTERED AT 09:14:17 ON 21 DEC 2003

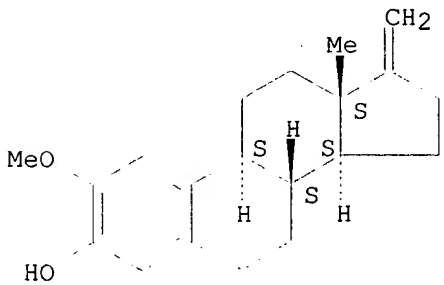
=> d bib abs hitstr l6

L6 ANSWER 1 OF 1 USPATFULL on STN
AN 2002:157823 USPATFULL
TI Antiangiogenic agents
IN Agoston, Gregory E., Germantown, MD, UNITED STATES
Shah, Jamshed H., Brookeville, MD, UNITED STATES
Hunsucker, Kimberly A., Germantown, MD, UNITED STATES
Pribluda, Victor S., Silver Spring, MD, UNITED STATES
LaVallee, Theresa M., Rockville, MD, UNITED STATES
Green, Shawn J., Vienna, VA, UNITED STATES
Herbstritt, Christopher J., Rockville, VA, UNITED STATES
Zhan, Xiaoguo H., Montgomery Village, MD, UNITED STATES
Treston, Anthony M., Rockville, MD, UNITED STATES
PI US 2002082433 A1 20020627
AI US 2001-939208 A1 20010824 (9)
RLI Continuation-in-part of Ser. No. US 2001-933894, filed on 21 Aug 2001, PENDING Continuation-in-part of Ser. No. US 2000-641327, filed on 18 Aug 2000, PENDING
PRAI US 2000-253385P 20001127 (60)
US 2000-255302P 20001213 (60)
US 2001-278250P 20010323 (60)
DT Utility
FS APPLICATION
LREP John S. Pratt, KILPATRICK STOCKTON LLP, Suite 2800, 1100 Peachtree Street, Atlanta, GA, 30309-4530
CLMN Number of Claims: 92
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 2637
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Compositions and methods for treating mammalian disease characterized by undesirable angiogenesis by administering derivatives of 2-methoxyestradiol of the general formula: ##STR1##

wherein the variables are defined in the specification.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **431901-73-4P**
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)
RN 431901-73-4 USPATFULL
CN Estra-1,3,5(10)-trien-3-ol, 2-methoxy-17-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)
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FILE COVERS 1907 - 21 Dec 2003  VOL 139 ISS 26
FILE LAST UPDATED: 19 Dec 2003  (20031219/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


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L7   ANSWER 1 OF 2  HCAPLUS  COPYRIGHT 2003 ACS on STN
AN   2002:488275  HCAPLUS
DN   137:47357
ED   Entered STN:  28 Jun 2002
TI   Preparation of 2-methoxyestradiol derivatives as antiangiogenic agents
IN   Agoston, Gregory E.; Shah, Jamshed H.; Hunsucker, Kimberly A.; Pribluda,
     Victor S.; Lavallee, Theresa M.; Green, Shawn J.; Herbstritt, Christopher
     J.; Zhan, Xiaoguo H.; Treston, Anthony M.
PA   USA
SO   U.S. Pat. Appl. Publ., 37 pp., Cont.-in-part of U. S. Ser. No. 933,894.
     CODEN: USXXCO
DT   Patent
LA   English
IC   ICM  C07J041-00
     ICS  C07J043-00; C07J001-00; A61K031-704; A61K031-58; A61K031-56;
          C07C247-00; A61K031-655; C07J009-00
NCL  552544000
CC   32-3 (Steroids)
     Section cross-reference(s): 1
FAN.CNT 2
     PATENT NO.         KIND  DATE          APPLICATION NO.  DATE
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PI   US 2002082433      A1    20020627      US 2001-939208   20010824
PRAI US 2000-641327     A2    20000818
     US 2000-253385P    P     20001127
     US 2000-255302P    P     20001213
     US 2001-278250P    P     20010323
     US 2001-933894     A2    20010821
OS   MARPAT 137:47357
GI
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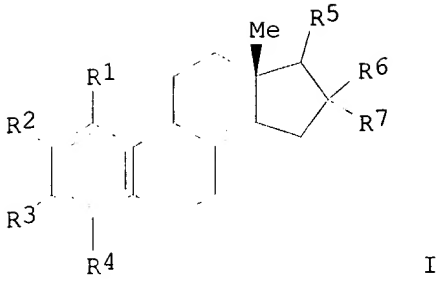

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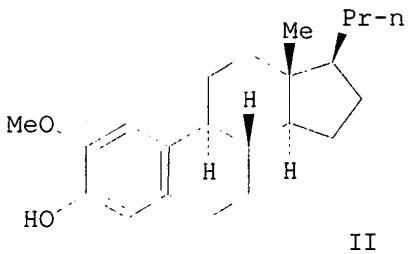

II

AB 2-Methoxyestradiol derivs. of formula I [R1, R4 = H, halo, CN, alkyl, OH, NH2, etc.; R2 = N3, CN, OMe, alkenyl, alkynyl, alkoxy, NH2, etc.; R3 = OH, OAc; R5 = alkyl, alkenyl, (di)alkylamino, OH, alkylene, etc.; R6, R7 = H, alkyl, alkenyl, alkynyl, halo, etc.] are prepared for treating mammalian disease characterized by undesirable angiogenesis. Thus, II was prepared from 2-methoxyestradiol and propyltriphenylphosphonium bromide. The IC50 of II against MDA-MB-231 breast tumor cells was 51.31 μM.

ST methoxyestradiol deriv prepn antiangiogenic; estradiol deriv prepn antiangiogenic; antitumor methoxyestradiol deriv prepn; antimitotic methoxyestradiol deriv prepn

IT Structure-activity relationship
(antitumor; preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT Mitosis
(inhibitors; preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT Angiogenesis inhibitors
Antitumor agents
Human
Mammary gland, neoplasm
Neoplasm
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT 362-07-2, 2-Methoxyestradiol
RL: PAC (Pharmacological activity); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT 53-63-4P, Estra-1,3,5(10)-trien-3-ol 6301-87-7P 431901-72-3P
431901-73-4P 431901-75-6P 431901-77-8P 431901-91-6P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT 1818-12-8P 4953-96-2P 6298-51-7P 6599-97-9P 7291-57-8P
10332-20-4P 32162-96-2P 41259-43-2P 94440-60-5P 165619-07-8P
165881-61-8P 229486-18-4P 431901-68-7P 431901-69-8P 431901-70-1P
431901-71-2P 431901-74-5P 431901-78-9P 431901-87-0P 431901-90-5P
431901-92-7P 431901-93-8P 431901-94-9P 431901-95-0P 431901-96-1P
431901-97-2P 431901-98-3P 431901-99-4P 431902-00-0P 431902-01-1P
431902-02-2P 431902-03-3P 431902-04-4P 431902-05-5P 431902-06-6P
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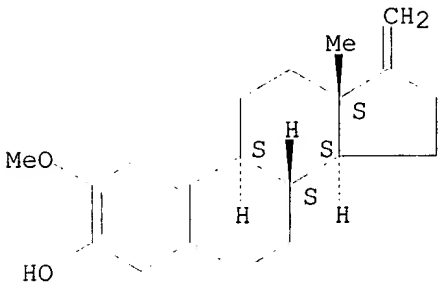
438044-35-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT 53-16-7, Estrone, reactions 106-95-6, Allyl bromide, reactions
1779-51-7, Butyltriphenylphosphonium bromide 4784-77-4, Crotyl bromide
5815-08-7 6228-47-3, Propyltriphenylphosphonium bromide
RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)
IT 26356-54-7P 26357-07-3P 93949-26-9P 431901-79-0P 431901-81-4P
431901-82-5P 431901-83-6P 431901-84-7P 431901-85-8P 431901-89-2P
438044-31-6P 438044-32-7P 438044-33-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)
IT **431901-73-4P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)
RN 431901-73-4 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 2-methoxy-17-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 2002:408687 HCAPLUS
DN 137:6309
ED Entered STN: 31 May 2002
TI Preparation of 2-methoxyestradiol analogs as antiangiogenic agents
IN Agoston, Gregory; Shah, Jamshed H.; Hunsucker, Kimberly A.; Pribluda, Victor; Lavallee, Theresa M.; Green, Shawn J.; Herbstritt, Christopher J.; Zhan, Xiaoguo H.; Treston, Anthony
PA Entremed, Inc., USA
SO PCT Int. Appl., 86 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07J001-00
CC 32-3 (Steroids)
Section cross-reference(s): 1, 2, 63
FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002042319	A2	20020530	WO 2001-US26490	20010824
WO 2002042319	A3	20030313		

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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2001088386	A5	20020603	AU 2001-88386	20010824
EP 1343803	A2	20030917	EP 2001-968112	20010824

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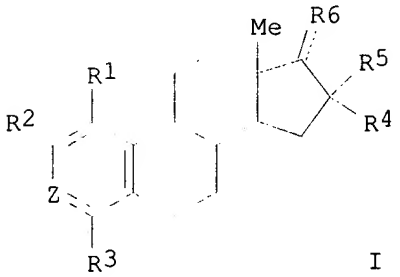
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
PRAI US 2000-253385P P 20001127
US 2000-255302P P 20001213
US 2001-278250P P 20010323
US 2001-933894 A 20010821
WO 2001-US26490 W 20010824
OS MARPAT 137:6309
GI



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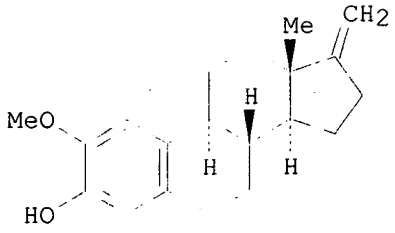

II

AB 2-Methoxyestradiol analogs, such as I [R1, R3 = H, halo, CN, alkyl, OH, CH2OH, NH2, alkylamino; R2 = N3, CN, C.tplbond.CR, C=CHR, C.tplbond.CH, OR, amino; R = H, alkyl; Z = COH, COAc; dashed bond = single bond or double bond; R6 = H, OH, O, oxime, amino, alkyl, alkenyl; R4, R5 = H, alkyl, alkenyl, alkynyl], were prepared for treating mammalian disease characterized by undesirable angiogenesis. Thus, 2-methoxyestradiol analog II was prepared by the reaction of methyltriphenylphosphonium bromide and 2-methoxyestrone. In vitro evaluation against MDA-MB-231 breast tumor cells and HUVEC endothelial cells, II showed IC50 0.24±0 and 0.19±0.19 resp.

ST methoxyestradiol deriv prepn antiangiogenic antitumor; estradiol methoxy deriv prepn antiangiogenic antitumor

IT Cell proliferation
(inhibition; preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT Mammary gland, neoplasm
(inhibitors; preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT Antitumor agents
(mammary gland; preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT Angiogenesis inhibitors
Human
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT Estrogens
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT 53-63-4P, Estra-1,3,5(10)-trien-3-ol 431901-72-3P **431901-73-4P**
431901-75-6P 431901-77-8P 431901-83-6P 431901-89-2P 431901-91-6P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT 1818-12-8P 4953-96-2P 6298-51-7P 6301-87-7P 6599-97-9P
7291-57-8P 10332-20-4P 32162-96-2P 41259-43-2P 94440-60-5P
165619-07-8P 165881-61-8P 192062-02-5P 229486-18-4P 431901-68-7P

431901-69-8P 431901-70-1P 431901-71-2P 431901-74-5P 431901-76-7P
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

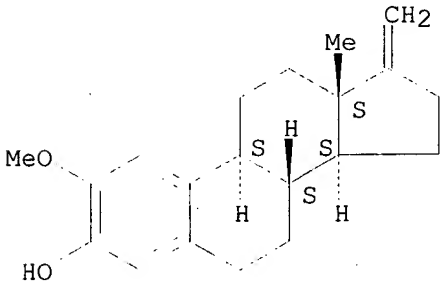
IT 53-16-7, Estrone, reactions 64-18-6, Formic acid, reactions 100-39-0, Benzyl bromide 106-95-6, Allyl bromide, reactions 362-07-2, 2-Methoxyestradiol 1530-32-1, Ethyl triphenylphosphonium bromide 1779-49-3, Methyl triphenylphosphonium bromide 1779-51-7, Butyl triphenylphosphonium bromide 4784-77-4, Crotyl bromide 5815-08-7, tert-Butoxy bis(dimethylamino)methane 6228-47-3, Propyl triphenylphosphonium bromide 17640-15-2, Methyl cyanoformate
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT 26356-54-7P 26357-07-3P 93949-26-9P 431901-79-0P 431901-80-3P
431901-81-4P 431901-85-8P 431901-90-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT **431901-73-4P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

RN 431901-73-4 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 2-methoxy-17-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 19 DEC 2003 HIGHEST RN 628722-21-4
DICTIONARY FILE UPDATES: 19 DEC 2003 HIGHEST RN 628722-21-4

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when

conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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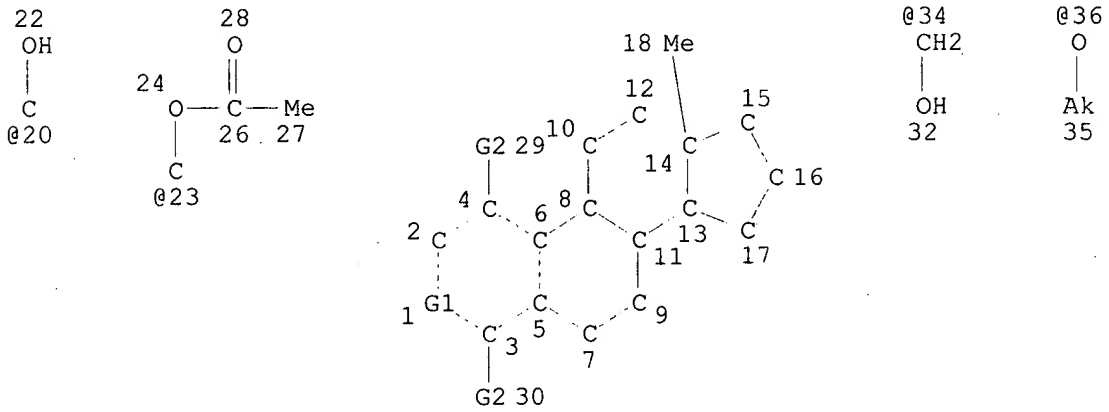

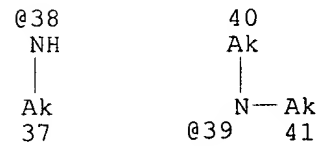

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CONNECT IS M1 RC AT 16
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 36

STEREO ATTRIBUTES: NONE
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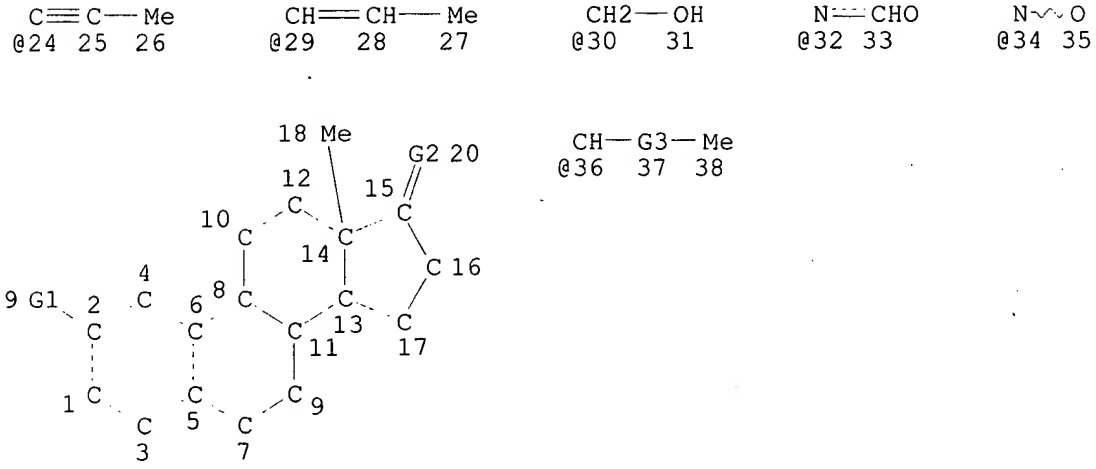
L24 STR



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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 15
NUMBER OF NODES IS 35

STEREO ATTRIBUTES: NONE
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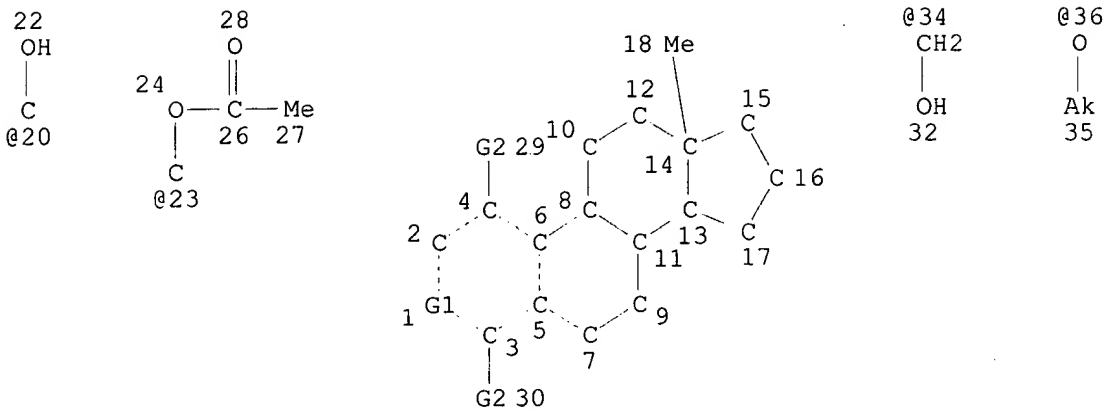
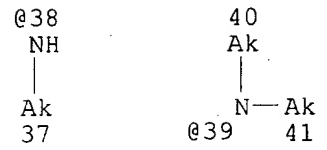
100.0% PROCESSED 76 ITERATIONS 10 ANSWERS
SEARCH TIME: 00.00.01

=> d sta que l32
L8 243537 SEA FILE=REGISTRY ABB=ON PLU=ON C5-C6-C6-C6/ES
L13 STR

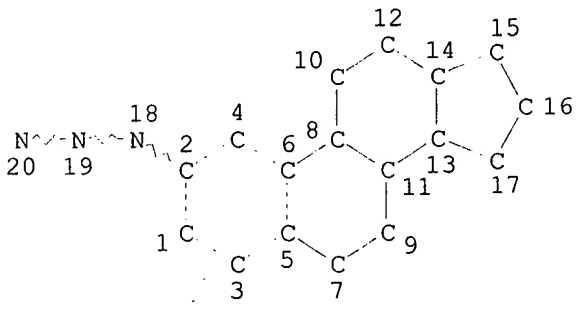




VAR G1=20/23
VAR G2=H/X/CN/AK/OH/34/NH2/36/38/39
NODE ATTRIBUTES:
CONNECT IS M1 RC AT 2
CONNECT IS M1 RC AT 15
CONNECT IS M1 RC AT 16
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 1
NUMBER OF NODES IS 36

STEREO ATTRIBUTES: NONE
L15 4643 SEA FILE=REGISTRY SUB=L8 CSS FUL L13
L30 STR



claim 91

NODE ATTRIBUTES:
CONNECT IS M1 RC AT 1
CONNECT IS M1 RC AT 3
CONNECT IS M1 RC AT 4
CONNECT IS M1 RC AT 15
CONNECT IS M1 RC AT 16
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 1
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE
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100.0% PROCESSED 9 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

=> d sta que l35
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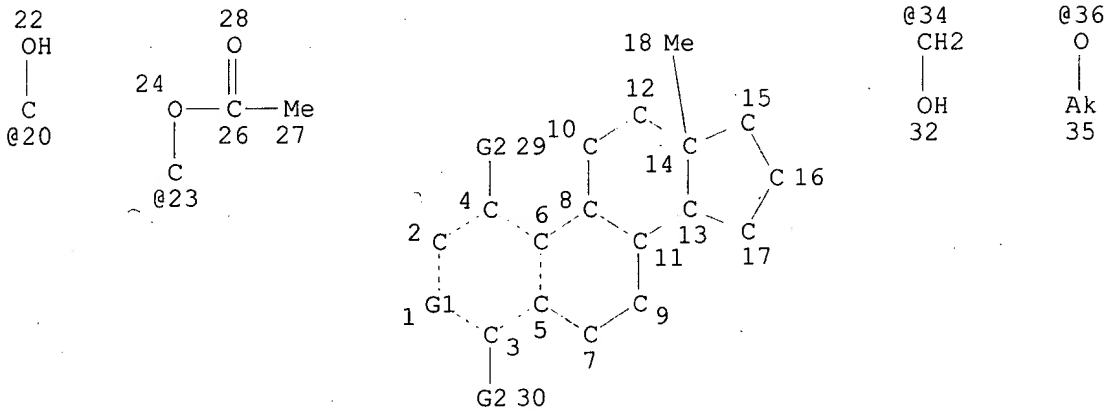
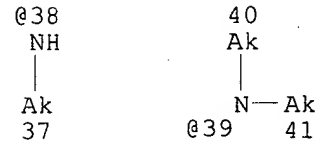
L13 STR

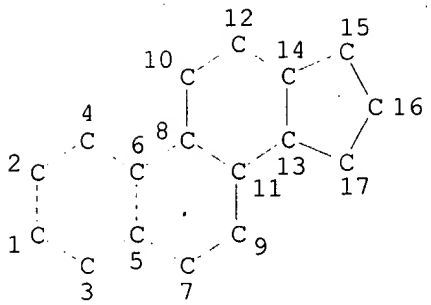




VAR G1=20/23
VAR G2=H/X/CN/AK/OH/34/NH2/36/38/39
NODE ATTRIBUTES:
CONNECT IS M1 RC AT 2
CONNECT IS M1 RC AT 15
CONNECT IS M1 RC AT 16
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 1
NUMBER OF NODES IS 36

STEREO ATTRIBUTES: NONE
L15 4643 SEA FILE=REGISTRY SUB=L8 CSS FUL L13
L33 STR

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NODE ATTRIBUTES:
CONNECT IS M1  RC AT   1
CONNECT IS M1  RC AT   3
CONNECT IS M1  RC AT   4
CONNECT IS M1  RC AT  16
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC   2
NUMBER OF NODES IS  17

STEREO ATTRIBUTES: NONE
L35           0 SEA FILE=REGISTRY SUB=L15 CSS FUL L33

100.0% PROCESSED   4643 ITERATIONS                          0 ANSWERS
SEARCH TIME: 00.00.01


=> d his 126-

     (FILE 'REGISTRY' ENTERED AT 09:15:35 ON 21 DEC 2003)
L26           10 S L24 CSS FUL SUB=L15
                 SAV L26 QAZI939D/A
L27            9 S L26 NOT L3
L28              STR
L29            0 S L28 CSS SAM SUB=L15
L30              STR L28
L31            0 S L30 CSS SAM SUB=L15
L32            0 S L30 CSS FUL SUB=L15
                 SAV L32 QAZI939E/A
L33              STR L30
L34            0 S L33 CSS SAM SUB=L15
L35            0 S L33 CSS FULL SUB=L15
                 SAV L35 QAZI939F/A

     FILE 'HCAOLD' ENTERED AT 09:46:24 ON 21 DEC 2003
L36            0 S L27

     FILE 'USPATFULL, USPAT2' ENTERED AT 09:46:29 ON 21 DEC 2003
L37            5 S L27

     FILE 'HCAPLUS' ENTERED AT 09:46:41 ON 21 DEC 2003
L38            9 S L27
L39            2 S L38 AND ENTREMED?/PA,CS
L40            3 S L38 AND (AGOSTON ? OR SHAH ? OR HUNSUCKER ? OR PRIBLUDA ? OR
L41            9 S L38-L40
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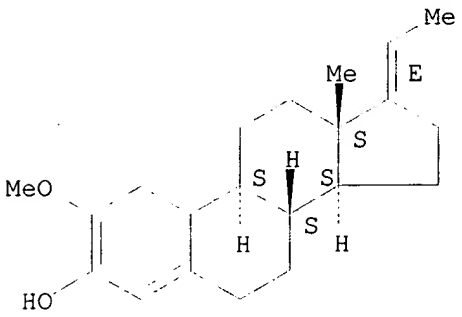
FILE 'REGISTRY' ENTERED AT 09:48:58 ON 21 DEC 2003

=> d ide can tot l27

L27 ANSWER 1 OF 9 REGISTRY COPYRIGHT 2003 ACS on STN
RN 594873-87-7 REGISTRY
CN 19-Norpregna-1,3,5(10),17(20)-tetraen-3-ol, 2-methoxy-, (17E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C21 H28 O2
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



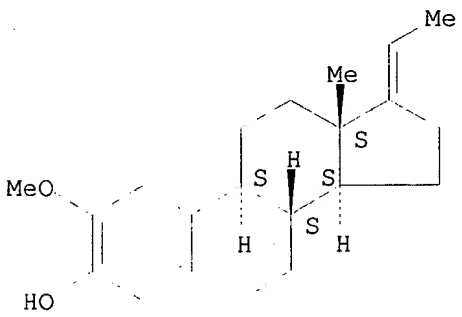
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:224972

L27 ANSWER 2 OF 9 REGISTRY COPYRIGHT 2003 ACS on STN
RN 431901-75-6 REGISTRY
CN 19-Norpregna-1,3,5(10),17(20)-tetraen-3-ol, 2-methoxy- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C21 H28 O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.
Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

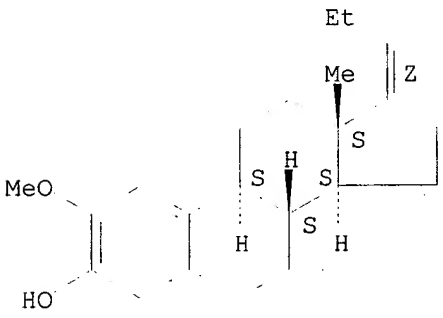
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:47357

REFERENCE 2: 137:6309

L27 ANSWER 3 OF 9 REGISTRY COPYRIGHT 2003 ACS on STN
RN 431901-72-3 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 2-methoxy-17-propylidene-, (17Z)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C22 H30 O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

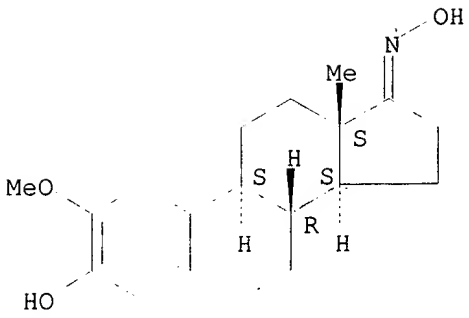
REFERENCE 1: 139:224972

REFERENCE 2: 137:47357

REFERENCE 3: 137:6309

L27 ANSWER 4 OF 9 REGISTRY COPYRIGHT 2003 ACS on STN
RN 431901-69-8 REGISTRY
CN Estra-1,3,5(10)-trien-17-one, 3-hydroxy-2-methoxy-, oxime (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C19 H25 N O3
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.
Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

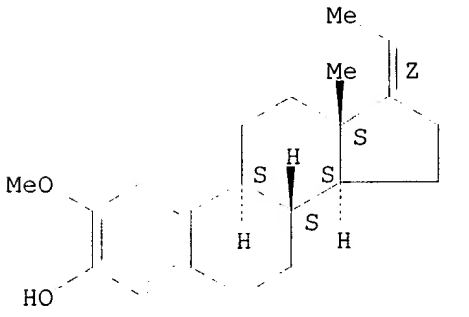
REFERENCE 1: 139:224972

REFERENCE 2: 137:47357

REFERENCE 3: 137:6309

L27 ANSWER 5 OF 9 REGISTRY COPYRIGHT 2003 ACS on STN
RN 229486-17-3 REGISTRY
CN 19-Norpregna-1,3,5(10),17(20)-tetraen-3-ol, 2-methoxy-, (17Z)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C21 H28 O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:370278

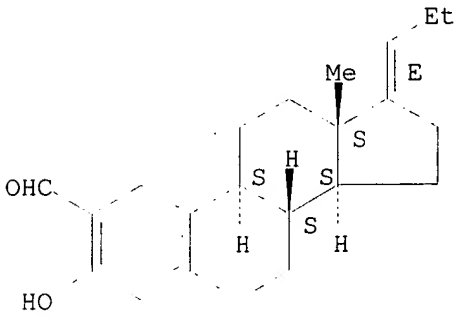
REFERENCE 2: 135:358085

REFERENCE 3: 133:350395

REFERENCE 4: 131:88083

L27 ANSWER 6 OF 9 REGISTRY COPYRIGHT 2003 ACS on STN
RN 208758-47-8 REGISTRY
CN Estra-1,3,5(10)-triene-2-carboxaldehyde, 3-hydroxy-17-propylidene-, (17E)-(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C22 H28 O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

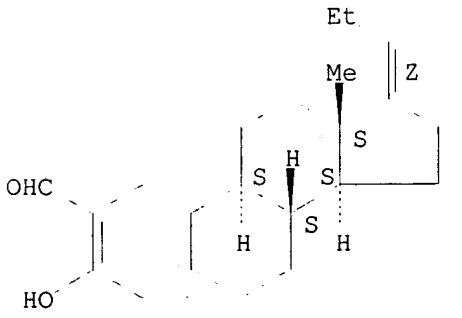
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:348841

REFERENCE 2: 129:54482

L27 ANSWER 7 OF 9 REGISTRY COPYRIGHT 2003 ACS on STN
RN 208758-28-5 REGISTRY
CN Estra-1,3,5(10)-triene-2-carboxaldehyde, 3-hydroxy-17-propylidene-, (17Z)-(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C22 H28 O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

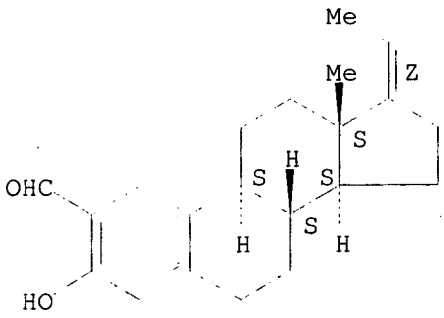
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:348841

REFERENCE 2: 129:54482

L27 ANSWER 8 OF 9 REGISTRY COPYRIGHT 2003 ACS on STN
RN 208758-27-4 REGISTRY
CN 19-Norpregna-1,3,5(10),17(20)-tetraene-2-carboxaldehyde, 3-hydroxy-, (17Z)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C21 H26 O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

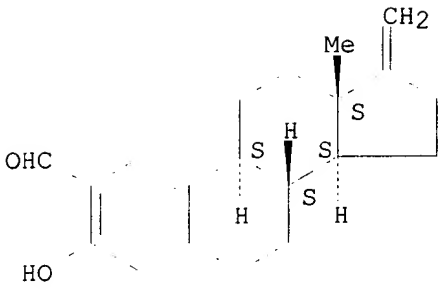
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:348841

REFERENCE 2: 129:54482

L27 ANSWER 9 OF 9 REGISTRY COPYRIGHT 2003 ACS on STN
RN 208758-26-3 REGISTRY
CN Estra-1,3,5(10)-triene-2-carboxaldehyde, 3-hydroxy-17-methylene- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C20 H24 O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:348841

REFERENCE 2: 129:54482

=> fil uspatall
FILE 'USPATFULL' ENTERED AT 09:49:31 ON 21 DEC 2003
CA INDEXING COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPAT2' ENTERED AT 09:49:31 ON 21 DEC 2003
CA INDEXING COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

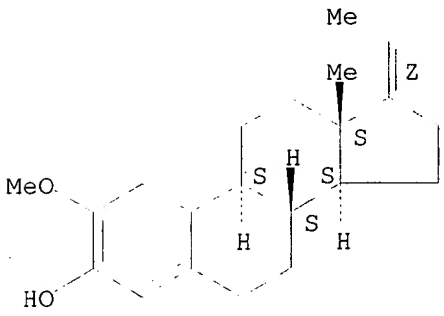
=> d l37 bib abs hitstr tot

L37 ANSWER 1 OF 5 USPATFULL on STN
AN 2003:226354 USPATFULL
TI 2-substituted pregna-1,3,5(10) triene and chola-1,3,5(10) triene derivatives and their biological activity
IN Hesse, Robert Henry, Winchester, MA, UNITED STATES
Setty, Sundara Katugam Srinivasasetty, Cambridge, MA, UNITED STATES
Pechet, Maurice Murdoch, Cambridge, MA, UNITED STATES
Gile, Michael, Methuen, MA, UNITED STATES
PI US 2003158167 A1 20030821
AI US 2003-275257 A1 20030313 (10)
WO 2001-GB2103 20010511
DT Utility
FS APPLICATION
LREP BACON & THOMAS, PLLC, 625 SLATERS LANE, FOURTH FLOOR, ALEXANDRIA, VA, 22314
CLMN Number of Claims: 13
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 978
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Compounds of formula (I) in which: R.sup.1 represents a hydrogen atom or an O-protecting group; R.sup.2 represents a hydroxyl, lower alkoxy, carboxaldehyde, lower alk-1-enyl or hydroxy- or lower alkoxy-substituted lower alkyl group; R.sup.3 represents a methyl group having α- or β-configuration; X represents a C.sub.1-3 alkylene group or a valence bond; Y represents a carboxaldehyde group or a group of formula --C(R.sup.4)(R.sup.5)OR.sup.1 where R.sup.1 is as defined above and R.sup.4 and R.sup.5, which may be the same or different, are each selected from hydrogen atoms, alkyl, alkenyl and alkynyl groups such that the total carbon content of R.sup.4 and R.sup.5 does not exceed

three atoms, with the proviso that X is a valence bond when both R.sup.4 and R.sup.5 are other than hydrogen; and the dotted line signifies that a double bond may optionally be present at the 16(17)-position exhibit potent cell modulating activity, including antiproliferative and antiangiogenic effects.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **229486-17-3P**
(preparation of 2-substituted pregnatriene and cholatriene derivs. with antiproliferative and antiangiogenic activity)
RN 229486-17-3 USPATFULL
CN 19-Norpregna-1,3,5(10),17(20)-tetraen-3-ol, 2-methoxy-, (17Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

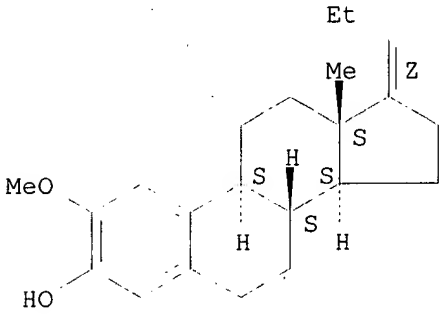


L37 ANSWER 2 OF 5 USPATFULL on STN
AN 2002:157823 USPATFULL
TI Antiangiogenic agents
IN Agoston, Gregory E., Germantown, MD, UNITED STATES
Shah, Jamshed H., Brookeville, MD, UNITED STATES
Hunsucker, Kimberly A., Germantown, MD, UNITED STATES
Pribluda, Victor S., Silver Spring, MD, UNITED STATES
LaVallee, Theresa M., Rockville, MD, UNITED STATES
Green, Shawn J., Vienna, VA, UNITED STATES
Herbstritt, Christopher J., Rockville, VA, UNITED STATES
Zhan, Xiaoguo H., Montgomery Village, MD, UNITED STATES
Treston, Anthony M., Rockville, MD, UNITED STATES
PI US 2002082433 A1 20020627
AI US 2001-939208 A1 20010824 (9)
RLI Continuation-in-part of Ser. No. US 2001-933894, filed on 21 Aug 2001, PENDING Continuation-in-part of Ser. No. US 2000-641327, filed on 18 Aug 2000, PENDING
PRAI US 2000-253385P 20001127 (60)
US 2000-255302P 20001213 (60)
US 2001-278250P 20010323 (60)
DT Utility
FS APPLICATION
LREP John S. Pratt, KILPATRICK STOCKTON LLP, Suite 2800, 1100 Peachtree Street, Atlanta, GA, 30309-4530
CLMN Number of Claims: 92
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 2637
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Compositions and methods for treating mammalian disease characterized by undesirable angiogenesis by administering derivatives of 2-methoxyestradiol of the general formula: ##STR1##

wherein the variables are defined in the specification.

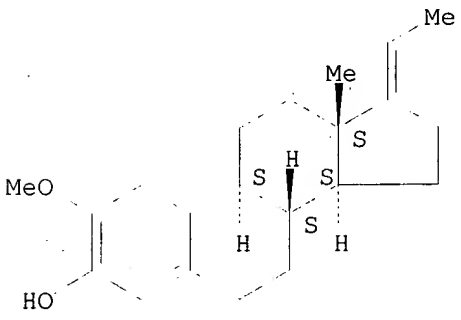
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **431901-72-3P 431901-75-6P**
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)
RN 431901-72-3 USPATFULL
CN Estra-1,3,5(10)-trien-3-ol, 2-methoxy-17-propylidene-, (17Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



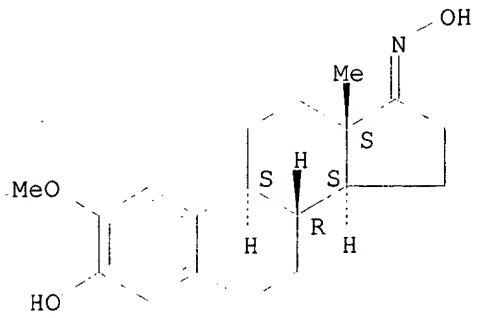
RN 431901-75-6 USPATFULL
CN 19-Norpregna-1,3,5(10),17(20)-tetraen-3-ol, 2-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



IT **431901-69-8P**
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)
RN 431901-69-8 USPATFULL
CN Estra-1,3,5(10)-trien-17-one, 3-hydroxy-2-methoxy-, oxime (9CI) (CA INDEX NAME)

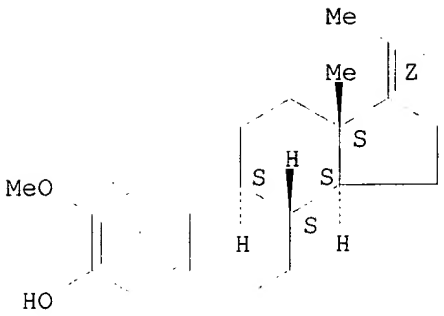
Absolute stereochemistry.
Double bond geometry unknown.



L37 ANSWER 3 OF 5 USPATFULL on STN
AN 2000:41031 USPATFULL
TI Estrone sulfamate inhibitors of estrone sulfatase, and associated pharmaceutical compositions and methods of use
IN Tanabe, Masato, Palo Alto, CA, United States
Peters, Richard H., San Jose, CA, United States
Chao, Wan-Ru, Sunnyvale, CA, United States
Shigeno, Kazuhiko, Saitama, CA, United States
PA SRI International, Menlo Park, CA, United States (U.S. corporation)
PI US 6046186 20000404
AI US 1997-997416 19971224 (8)
DT Utility
FS Granted
EXNAM Primary Examiner: Raymond, Richard L.; Assistant Examiner: Coleman, Brenda
LREP Reed, Dianne E.Reed & Associates
CLMN Number of Claims: 65
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 3007
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Novel compounds useful as inhibitors of estrone sulfatase are provided. The compounds have the structural formula (I) wherein r1 is an optional double bond, R.sup.1 and R.sup.2 are selected from the group consisting of hydrogen and lower alky, or together form a cyclic substituent (II) ##STR1## wherein Q is NH, O or CH.sub.2, and the other various substituents are as defined herein. Pharmaceutical compositions and methods for using the compounds of formula (I) to treat estrogen-dependent disorders are provided as well.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **229486-17-3P**
(preparation of estrone sulfamates as inhibitors of estrone sulfatase)
RN 229486-17-3 USPATFULL
CN 19-Norpregna-1,3,5(10),17(20)-tetraen-3-ol, 2-methoxy-, (17Z)- (9CI) (CA INDEX NAME)

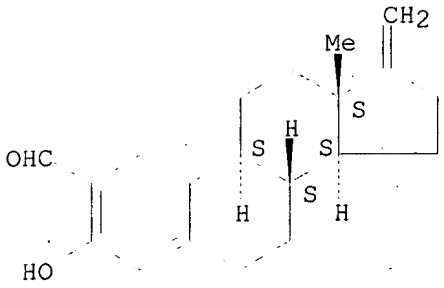
Absolute stereochemistry.
Double bond geometry as shown.



L37 ANSWER 4 OF 5 USPATFULL on STN
AN 1999:7375 USPATFULL
TI Steroid inhibitors of estrone sulfatase and associated pharmaceutical compositions and methods of use
IN Tanabe, Masato, Palo Alto, CA, United States
Peters, Richard H., San Jose, CA, United States
Chao, Wan-Ru, Sunnyvale, CA, United States
Shigeno, Kazuhiko, Mountain View, CA, United States
PA SRI International, Menlo Park, CA, United States (U.S. corporation)
PI US 5861388 19990119
AI US 1997-1601 19971231
RLI Division of Ser. No. US 1997-794229, filed on 29 Jan 1997, now patented, Pat. No. US 5763432
DT Utility
FS Granted
EXNAM Primary Examiner: Dees, Jose G.; Assistant Examiner: Bodio, Barbara
LREP Reed, Dianne E.Bozicevic & Reed LLP
CLMN Number of Claims: 22
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 1778
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Novel compounds useful as inhibitors of estrone sulfatase are provided. The compounds have the structural formula (I) ##STR1## wherein X and Y, or Y and Z, form an oxathiazine dioxide ring or a dihydro-oxathiazine dioxide ring, and the other various substituents are as defined herein. Pharmaceutical compositions and methods for using the compounds of formula (I) to treat estrogen-dependent disorders are provided as well.

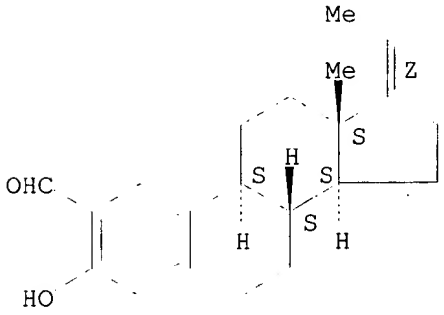
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **208758-26-3P 208758-27-4P 208758-28-5P**
208758-47-8P
(preparation of steroid inhibitors of estrone sulfatase)
RN 208758-26-3 USPATFULL
CN Estra-1,3,5(10)-triene-2-carboxaldehyde, 3-hydroxy-17-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



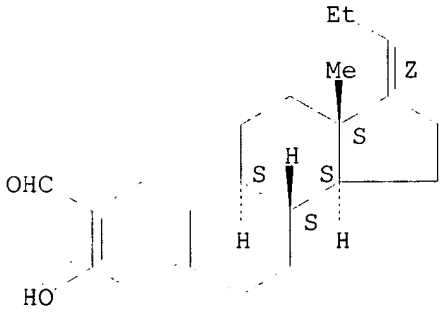
RN 208758-27-4 USPATFULL
CN 19-Norpregna-1,3,5(10),17(20)-tetraene-2-carboxaldehyde, 3-hydroxy-, (17Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



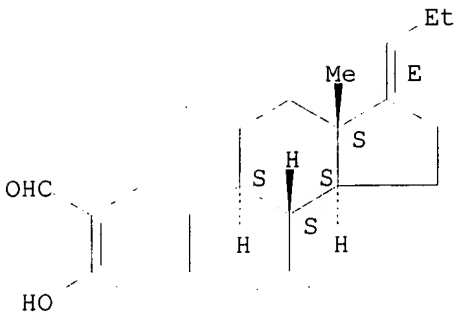
RN 208758-28-5 USPATFULL
CN Estra-1,3,5(10)-triene-2-carboxaldehyde, 3-hydroxy-17-propylidene-, (17Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 208758-47-8 USPATFULL
CN Estra-1,3,5(10)-triene-2-carboxaldehyde, 3-hydroxy-17-propylidene-, (17E)- (9CI) (CA INDEX NAME)

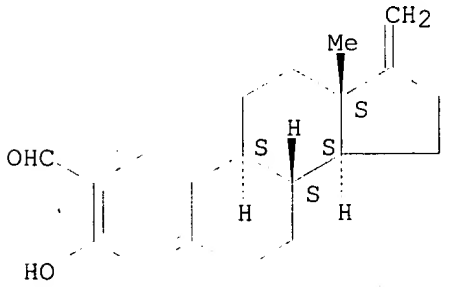
Absolute stereochemistry.
Double bond geometry as shown.



L37 ANSWER 5 OF 5 USPATFULL on STN
AN 1998:65215 USPATFULL
TI Steriod inhibitors of estrone sulfatase and associated pharmaceutical compositions and methods of use
IN Tanabe, Masato, Palo Alto, CA, United States
Peters, Richard H., San Jose, CA, United States
Chao, Wan-Ru, Sunnyvale, CA, United States
Shigeno, Kazuhiko, Mountain View, CA, United States
PA SRI International, Menlo Park, CA, United States (U.S. corporation)
PI US 5763432 19980609
AI US 1997-794229 19970129 (8)
DT Utility
FS Granted
EXNAM Primary Examiner: Dees, Jose G.; Assistant Examiner: Badio, Barbara
LREP Reed, Dianne E.Bozicevic & Reed LLP
CLMN Number of Claims: 13
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 1700
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Novel compounds useful as inhibitors of estrone sulfatase are provided. The compounds have the structural formula (I) ##STR1## wherein X and Y, or Y and Z, form an oxathiazine dioxide ring or a dihydro-oxathiazine dioxide ring, and the other various substituents are as defined herein. Pharmaceutical compositions and methods for using the compounds of formula (I) to treat estrogen-dependent disorders are provided as well.

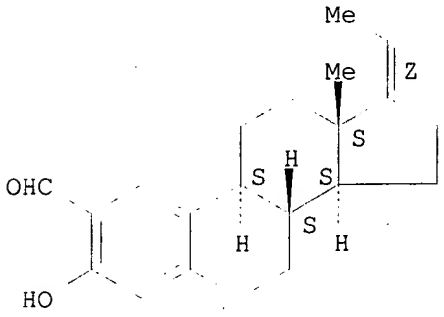
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **208758-26-3P 208758-27-4P 208758-28-5P**
208758-47-8P
(preparation of steroid inhibitors of estrone sulfatase)
RN 208758-26-3 USPATFULL
CN Estra-1,3,5(10)-triene-2-carboxaldehyde, 3-hydroxy-17-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



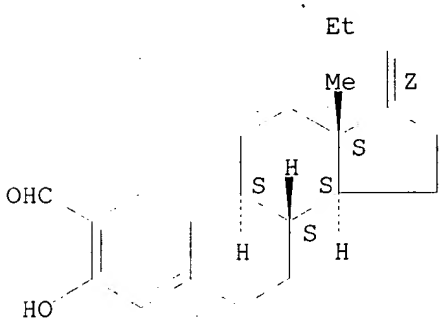
RN 208758-27-4 USPATFULL
CN 19-Norpregna-1,3,5(10),17(20)-tetraene-2-carboxaldehyde, 3-hydroxy-, (17Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



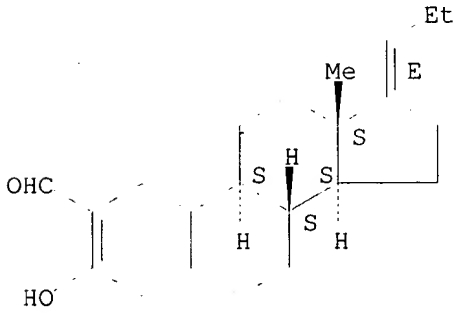
RN 208758-28-5 USPATFULL
CN Estra-1,3,5(10)-triene-2-carboxaldehyde, 3-hydroxy-17-propylidene-, (17Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 208758-47-8 USPATFULL
CN Estra-1,3,5(10)-triene-2-carboxaldehyde, 3-hydroxy-17-propylidene-, (17E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



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L41  ANSWER 1 OF 9  HCAPLUS  COPYRIGHT 2003 ACS on STN
AN   2003:719252  HCAPLUS
DN   139:224972
ED   Entered STN:  14 Sep 2003
TI   Synthesis of 2-methoxyestradiol derivatives and uses as antiangiogenic
     agents
IN   Lavallee, Theresa M.; Pribluda, Victor S.; Simons,
     Jonathan; Mabjeesh, Nicola; Giannakakou, Paraskevi
PA   Entremed, Inc., USA
SO   PCT Int. Appl., 77 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
IC   ICM  A61K
CC   2-4 (Mammalian Hormones)
     Section cross-reference(s): 32
FAN.CNT 1
     PATENT NO.        KIND  DATE          APPLICATION NO.  DATE
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PI   WO 2003073985     A2    20030912      WO 2003-US5898   20030227
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SC, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT,
             TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ,
             MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
             CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
             PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,
             NE, SN, TD, TG
PRAI US 2002-361267P   P    20020301
AB   Compns. and methods for treating mammalian disease characterized by
     undesirable angiogenesis and for controlling a number of angiogenesis-related
     events, conditions, or substances, by administering derivs. of
     2-methoxyestradiol of general formula (I) wherein the variables are
     defined in the specification.
```

ST estrogen methoxyestradiol analogs angiogenesis inhibitor VEGF DR5 HIFalpha

IT Apoptosis
(2-ME2-induced; synthesis of 2-methoxyestradiol derivs. and uses as antiangiogenic agents)

IT Cytokine receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(DR5 (death receptor 5); synthesis of 2-methoxyestradiol derivs. and uses as antiangiogenic agents)

IT Transcription factors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(HIF-1α (hypoxia-inducible factor 1α); synthesis of 2-methoxyestradiol derivs. and uses as antiangiogenic agents)

IT Blood vessel
(endothelium; synthesis of 2-methoxyestradiol derivs. and uses as antiangiogenic agents)

IT Transcriptional regulation
(of HIF-1α, 2-ME2-inhibited; synthesis of 2-methoxyestradiol derivs. and uses as antiangiogenic agents)

IT Angiogenesis
Angiogenesis inhibitors
Human
(synthesis of 2-methoxyestradiol derivs. and uses as antiangiogenic agents)

IT Estrogens
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis of 2-methoxyestradiol derivs. and uses as antiangiogenic agents)

IT 127464-60-2, Vascular Endothelial Growth Factor
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(synthesis of 2-methoxyestradiol derivs. and uses as antiangiogenic agents)

IT 362-07-2DP, 2-Methoxyestradiol, derivs. and analogs 362-07-2P, 2-Methoxyestradiol
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of 2-methoxyestradiol derivs. and uses as antiangiogenic agents)

IT 50-00-0, Formaldehyde, reactions 50-28-2D, Estradiol, derivs. and analogs 53-16-7, Estrone, reactions 64-18-6, Formic acid, reactions 64-19-7, Acetic acid, reactions 67-68-5, Methyl sulfoxide, reactions 68-12-2, DMF, reactions 71-36-3, 1-Butanol, reactions 75-09-2, Methylene chloride, reactions 79-37-8, Oxalyl chloride 100-39-0, Benzyl bromide 106-95-6, Allyl bromide, reactions 109-99-9, THF, reactions 111-46-6, Diethylene glycol, reactions 121-44-8, Triethylamine, reactions 141-78-6, Ethyl acetate, reactions 302-01-2, Hydrazine, reactions 362-08-3, 2-Methoxyestrone 362-08-3D, 2-Methoxyestrone, olefin analogs 584-08-7, Potassium carbonate 1157-87-5, AH3 1530-32-1, Ethyl triphenylphosphonium bromide 1779-49-3, Methyltriphenylphosphonium bromide 1779-51-7, Butyl triphenylphosphonium bromide 4111-54-0, Lithium diisopropyl amide 4784-77-4, Crotyl bromide 5815-08-7, tert-Butoxy bis(dimethylamino)methane 6228-47-3, Propyl triphenylphosphonium bromide 7447-41-8, Lithium chloride, reactions 7632-00-0, Sodium nitrite 7693-26-7, Potassium hydride 16853-85-3, Lithium aluminum hydride 17455-13-9, 18-Crown-6 17640-15-2, Methyl cyanoformate 41233-93-6, Potassium-tert-amylate 431901-79-0 431901-81-4 431901-84-7 431901-85-8 431901-89-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of 2-methoxyestradiol derivs. and uses as antiangiogenic agents)

IT 53-63-4P, Estra-1,3,5(10)-trien-3-ol

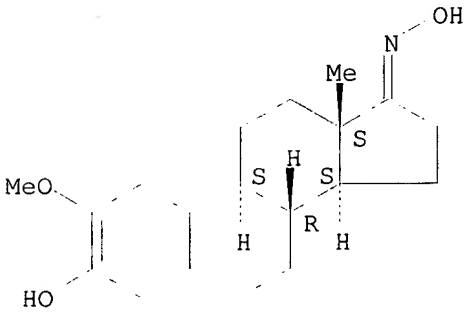
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of 2-methoxyestradiol derivs. and uses as antiangiogenic agents)

IT 362-07-2DP, 2-Methoxyestradiol, alkyl analogs 4953-96-2P 6298-51-7P 6301-87-7P 6599-97-9P 7291-57-8P 10332-20-4P 26356-54-7DP, alkyl derivs 26356-54-7DP, alkyl derivs. 26356-54-7P 26357-07-3DP, 16α-alkyl derivs. 26357-07-3P 32162-96-2P 34111-53-0P 93949-26-9P 165619-07-8P 229486-18-4P 431901-68-7P **431901-69-8P** 431901-70-1P 431901-71-2P **431901-72-3P** 431901-77-8P 431901-78-9P 431901-80-3DP, alkyl derivs. 431901-89-2DP, alkyl analogs 431901-90-5P 431901-91-6P 431901-92-7P 431901-93-8P 431901-98-3P 431901-99-4P 431902-01-1P 431902-02-2P 431902-03-3P 431902-04-4P 431902-05-5P 431902-06-6P 431902-09-9P 438044-30-5P 464924-32-1P 594873-85-5P 594873-86-6P **594873-87-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of 2-methoxyestradiol derivs. and uses as antiangiogenic agents)

IT **431901-69-8P 431901-72-3P 594873-87-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of 2-methoxyestradiol derivs. and uses as antiangiogenic agents)

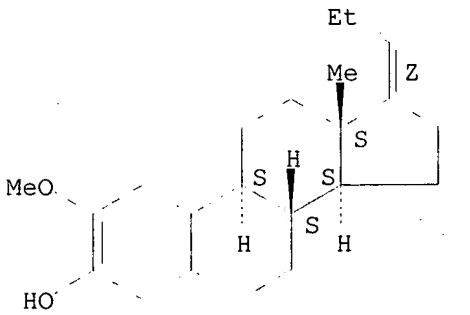
RN 431901-69-8 HCAPLUS
CN Estra-1,3,5(10)-trien-17-one, 3-hydroxy-2-methoxy-, oxime (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



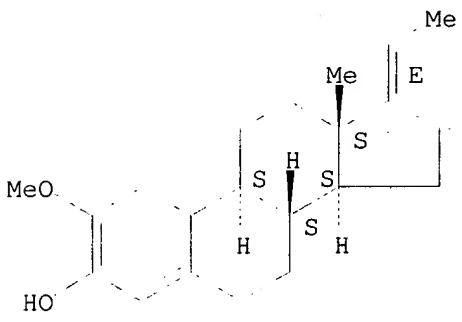
RN 431901-72-3 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 2-methoxy-17-propylidene-, (17Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 594873-87-7 HCAPLUS
CN 19-Norpregna-1,3,5(10),17(20)-tetraen-3-ol, 2-methoxy-, (17E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L41 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 2002:935062 HCAPLUS
DN 138:348841
ED Entered STN: 10 Dec 2002
TI Steroidal oxathiazine inhibitors of estrone sulfatase
AU Peters, Richard H.; Chao, Wan-Ru; Sato, Barbara; Shigeno, Kazuhiko; Zaveri, Nurulain T.; Tanabe, Masato
CS Life Science Division, SRI International, Menlo Park, CA, 94025, USA
SO Steroids (2003), 68(1), 97-110
CODEN: STEDAM; ISSN: 0039-128X
PB Elsevier Science Inc.
DT Journal
LA English
CC 2-4 (Mammalian Hormones)
Section cross-reference(s): 1, 7
OS CASREACT 138:348841
AB The presence of estrone sulfatase in breast tumors and the high levels of circulating estrone sulfate may contribute the major portion of estrogen synthesized locally in breast tissues through conversion of estrone sulfate to estrone by the enzyme. Using inhibitors of estrone sulfatase for the treatment of estrogen-dependent (estrogen receptor pos., ER+) breast cancer could be a very effective therapeutic strategy for the treatment of estrogen-dependent breast tumors in postmenopausal women. Therefore, the authors designed and synthesized several steroidal 2',3'-oxathiazines that inhibit estrone sulfatase and have greatly reduced estrogenic side effects. The authors' in vitro studies indicate that the oxathiazine compds. have inhibitory activity on estrone sulfatase in MCF-7 human breast cancer cells. These estrone sulfatase inhibitors (ESIs) also inhibit the growth of MCF-7 cells induced by estrone sulfate. In addition, the authors' in vivo expts. demonstrate that the authors' ESIs have moderate antitumor activity against MCF-7 breast cancer xenografts in Balb/c athymic nude mice. The synthesis and biol. activity of a number of these unique steroidal ESIs are described.
ST estrone sulfatase inhibitor breast cancer proliferation inhibition
IT Cell proliferation
(inhibition; steroidal oxathiazine inhibitors of estrone sulfatase in relation to synthesis and biol. activity in MCF-7 cells)
IT Antitumor agents
Double bond
Human
Mammary gland, neoplasm
(steroidal oxathiazine inhibitors of estrone sulfatase in relation to

synthesis and biol. activity in MCF-7 cells)

IT 53-16-7, Estrone, biological studies 481-97-0, Estrone sulfate
RL: ADV (Adverse effect, including toxicity); BSU (Biological study, unclassified); BIOL (Biological study)
(steroidal oxathiazine inhibitors of estrone sulfatase in relation to synthesis and biol. activity in MCF-7 cells)

IT 7732-18-5, Water, biological studies 9001-78-9, Alkaline phosphatase 59298-96-3, Sulfatase, estrone
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(steroidal oxathiazine inhibitors of estrone sulfatase in relation to synthesis and biol. activity in MCF-7 cells)

IT 208758-16-1P 208758-17-2P 208758-20-7P 208758-21-8P 208758-23-0P
208758-25-2P 208758-33-2P 208758-34-3P 208758-35-4P 208758-36-5P
208758-37-6P 208758-38-7P 208758-39-8P 208758-41-2P 208758-43-4P
208758-48-9P 208758-52-5P 208758-54-7P 519039-19-1P 519039-26-0P
519039-29-3P 519039-31-7P 519039-33-9P 519039-37-3P
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(steroidal oxathiazine inhibitors of estrone sulfatase in relation to synthesis and biol. activity in MCF-7 cells)

IT 6599-97-9P 13879-55-5P 13879-56-6P 31559-62-3P 123715-79-7P
137352-12-6P 208758-18-3P 208758-19-4P 208758-22-9P 208758-24-1P
208758-26-3P 208758-27-4P 208758-28-5P
208758-29-6P 208758-30-9P 208758-31-0P 208758-32-1P 208758-40-1P
208758-42-3P **208758-47-8P** 208758-51-4P 208758-53-6P
519039-17-9P 519039-25-9P 519039-28-2P 519039-30-6P 519039-34-0P
519039-35-1P 519039-36-2P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(steroidal oxathiazine inhibitors of estrone sulfatase in relation to synthesis and biol. activity in MCF-7 cells)

IT 50-28-2, Estra-1,3,5(10)-triene-3,17-diol (17β)-, reactions
1189-71-5, Chlorosulfonyl isocyanate 4736-62-3 4954-12-5 18162-48-6, Tert-Butyldimethyl chlorosilane 34111-53-0 64215-82-3 99898-93-8
116627-20-4 120574-27-8 120574-28-9 185910-40-1 208758-46-7
208758-50-3 229486-09-3 229486-13-9 519039-16-8 519039-27-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(steroidal oxathiazine inhibitors of estrone sulfatase in relation to synthesis and biol. activity in MCF-7 cells)

RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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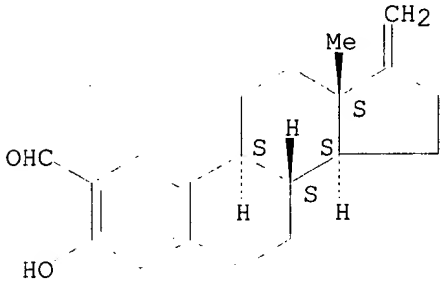
IT **208758-26-3P 208758-27-4P 208758-28-5P**
208758-47-8P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(steroidal oxathiazine inhibitors of estrone sulfatase in relation to synthesis and biol. activity in MCF-7 cells)

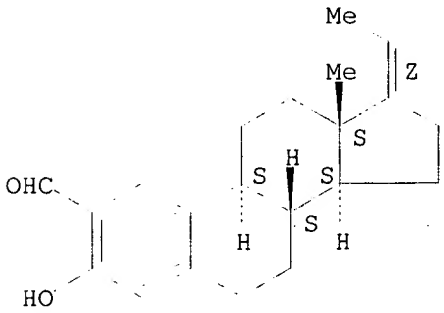
RN 208758-26-3 HCAPLUS
CN Estra-1,3,5(10)-triene-2-carboxaldehyde, 3-hydroxy-17-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



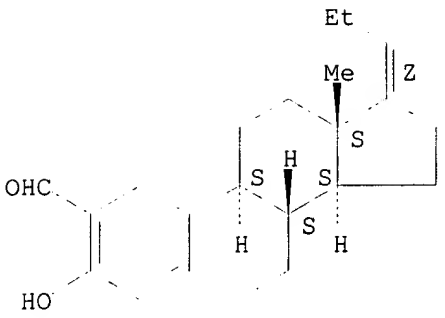
RN 208758-27-4 HCAPLUS
CN 19-Norpregna-1,3,5(10),17(20)-tetraene-2-carboxaldehyde, 3-hydroxy-, (17Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



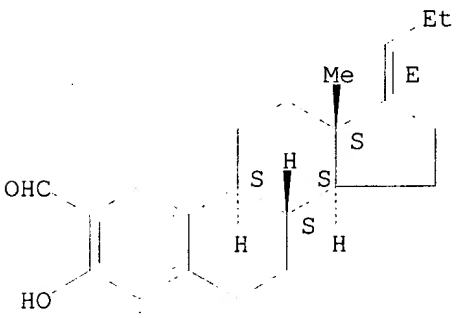
RN 208758-28-5 HCAPLUS
CN Estra-1,3,5(10)-triene-2-carboxaldehyde, 3-hydroxy-17-propylidene-, (17Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 208758-47-8 HCAPLUS
CN Estra-1,3,5(10)-triene-2-carboxaldehyde, 3-hydroxy-17-propylidene-, (17E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

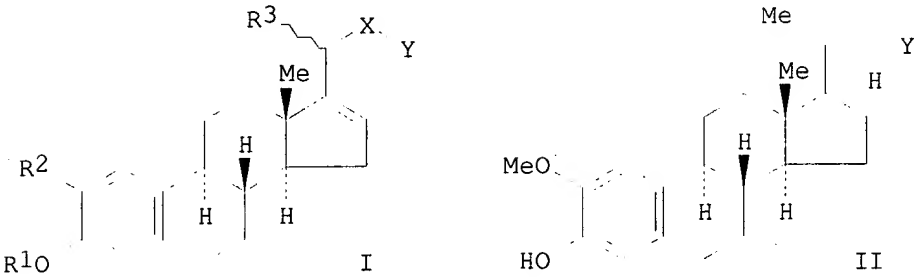


L41 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 2002:888569 HCAPLUS
DN 137:370278
ED Entered STN: 22 Nov 2002
TI Preparation of substituted pregna-1,3,5(10)-triene derivatives for pharmaceutical use
IN Hesse, Robert Henry; Setty, Sundara Katugam Srinivasasetty; Pechet, Maurice Murdoch; Gile, Michael
PA Marsden, John Christopher, UK; Research Institute for Medicine and Chemistry Inc.
SO PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM A61K031-56
ICS A61K031-575; C07J041-00; A61P035-00
CC 32-5 (Steroids)
Section cross-reference(s): 1, 2, 63
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002092100	A1	20021121	WO 2002-GB2210	20020513

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,

TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
PRAI US 2001-290013P P 20010511
OS MARPAT 137:370278
GI



AB Pregna-1,3,5(10)-triene derivs., such as I [R1 = H, hydroxy protecting group; R2 = OH, CHO, alkoxy, alkenyl, alkyl, etc.; R3 = α-, β-Me; X = C1-3 alkylene group, bond; Y = C(R4)(R5)NR6R7; R4, R5 = H, alkyl, alkenyl and alkynyl groups, such that the total carbon content of R4 and R5 does not exceed three atoms; R6 = H, aliphatic or araliph. organic group, acyl, etc.; C16-C17 = saturated, unsatd.], were prepared for a variety of therapeutic uses, such as modulating cell activity, including antiproliferative and antiangiogenic effects. Thus, pregna-1,3,5(10)-triene derivs. II (Y = NH2, NHCOMe) were prepared via a multistep synthetic series starting from 2-methoxy-3-[[tris(1-methylethyl)silyl]oxy]-estra-1,3,5(10)-trien-17-one and ethyltriphenylphosphonium bromide. Pharmaceutical compns. of the prepared compds. were discussed, but specific pharmaceutical activity testing data was not presented.

ST norpregnatriene prepn antiproliferative antiangiogenic agent

IT Mental disorder
(cognitive, treatment; preparation of substituted pregna-1,3,5(10)-triene derivs. for a variety of therapeutic uses)

IT Blood coagulation
Cognition
(disorder, treatment; preparation of substituted pregna-1,3,5(10)-triene derivs. for a variety of therapeutic uses)

IT Transplant and Transplantation
(graft-vs.-host reaction, treatment; preparation of substituted pregna-1,3,5(10)-triene derivs. for a variety of therapeutic uses)

IT Anti-inflammatory agents
Anticholesteremic agents
Antitumor agents
Cognition enhancers
Contraceptives
Immunomodulators
(preparation of substituted pregna-1,3,5(10)-triene derivs. for a variety of therapeutic uses)

IT Arthritis
(psoriatic arthritis, treatment; preparation of substituted pregna-1,3,5(10)-triene derivs. for a variety of therapeutic uses)

IT Mental disorder
(senile psychosis, treatment; preparation of substituted pregna-1,3,5(10)-triene derivs. for a variety of therapeutic uses)

IT Asthma
Autoimmune disease
Bone, disease
Hypercholesterolemia
Hyperplasia
Hypertension
Inflammation
Neoplasm
Rheumatoid arthritis
Skin, disease
Transplant rejection
(treatment; preparation of substituted pregna-1,3,5(10)-triene derivs. for a variety of therapeutic uses)

IT 4736-60-1, Ethyltriphenylphosphonium iodide 305812-67-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of substituted pregna-1,3,5(10)-triene derivs. for a variety of therapeutic uses)

IT **229486-17-3P** 305812-87-7P 305812-99-1P 372952-47-1P 372952-49-3P 372952-50-6P 475486-81-8P 475486-82-9P 475486-83-0P 475486-84-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of substituted pregna-1,3,5(10)-triene derivs. for a variety of therapeutic uses)

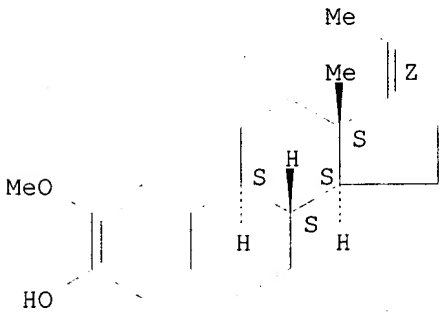
IT 475486-79-4P 475486-80-7P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted pregna-1,3,5(10)-triene derivs. for a variety of therapeutic uses)

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Christopher, M; WO 0068246 A 2000 HCAPLUS
(2) Christopher, M; WO 0185755 A 2001 HCAPLUS
(3) Cushman, M; JOURNAL OF MEDICINAL CHEMISTRY 1995, V38(12), P2041 HCAPLUS
(4) Jacques, P; US 3291690 A 1966

IT **229486-17-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of substituted pregna-1,3,5(10)-triene derivs. for a variety of therapeutic uses)

RN 229486-17-3 HCAPLUS
CN 19-Norpregna-1,3,5(10),17(20)-tetraen-3-ol, 2-methoxy-, (17Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

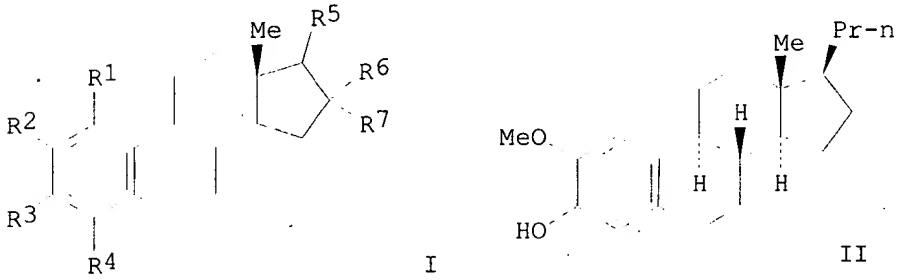


L41 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 2002:488275 HCAPLUS

DN 137:47357
ED Entered STN: 28 Jun 2002
TI Preparation of 2-methoxyestradiol derivatives as antiangiogenic agents
IN **Agoston, Gregory E.; Shah, Jamshed H.; Hunsucker, Kimberly A.; Pribluda, Victor S.; Lavallee, Theresa M.; Green, Shawn J.; Herbstritt, Christopher J.; Zhan, Xiaoguo H.; Treston, Anthony M.**
PA USA
SO U.S. Pat. Appl. Publ., 37 pp., Cont.-in-part of U. S. Ser. No. 933,894.
CODEN: USXXCO
DT Patent
LA English
IC ICM C07J041-00
ICS C07J043-00; C07J001-00; A61K031-704; A61K031-58; A61K031-56; C07C247-00; A61K031-655; C07J009-00
NCL 552544000
CC 32-3 (Steroids)
Section cross-reference(s): 1
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2002082433	A1	20020627	US 2001-939208	20010824
PRAI	US 2000-641327	A2	20000818		
	US 2000-253385P	P	20001127		
	US 2000-255302P	P	20001213		
	US 2001-278250P	P	20010323		
	US 2001-933894	A2	20010821		

OS MARPAT 137:47357
GI



AB 2-Methoxyestradiol derivs. of formula I [R1, R4 = H, halo, CN, alkyl, OH, NH2, etc.; R2 = N3, CN, OMe, alkenyl, alkynyl, alkoxy, NH2, etc.; R3 = OH, OAc; R5 = alkyl, alkenyl, (di)alkylamino, OH, alkylene, etc.; R6, R7 = H, alkyl, alkenyl, alkynyl, halo, etc.] are prepared for treating mammalian disease characterized by undesirable angiogenesis. Thus, II was prepared from 2-methoxyestradiol and propyltriphenylphosphonium bromide. The IC50 of II against MDA-MB-231 breast tumor cells was 51.31 μM.
ST methoxyestradiol deriv prepn antiangiogenic; estradiol deriv prepn antiangiogenic; antitumor methoxyestradiol deriv prepn; antimitotic methoxyestradiol deriv prepn
IT Structure-activity relationship
(antitumor; preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)
IT Mitosis
(inhibitors; preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)
IT Angiogenesis inhibitors

Antitumor agents
Human
Mammary gland, neoplasm
Neoplasm
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT 362-07-2, 2-Methoxyestradiol
RL: PAC (Pharmacological activity); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT 53-63-4P, Estra-1,3,5(10)-trien-3-ol 6301-87-7P **431901-72-3P**
431901-73-4P **431901-75-6P** 431901-77-8P 431901-91-6P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT 1818-12-8P 4953-96-2P 6298-51-7P 6599-97-9P 7291-57-8P
10332-20-4P 32162-96-2P 41259-43-2P 94440-60-5P 165619-07-8P
165881-61-8P 229486-18-4P 431901-68-7P **431901-69-8P**
431901-70-1P 431901-71-2P 431901-74-5P 431901-78-9P 431901-87-0P
431901-90-5P 431901-92-7P 431901-93-8P 431901-94-9P 431901-95-0P
431901-96-1P 431901-97-2P 431901-98-3P 431901-99-4P 431902-00-0P
431902-01-1P 431902-02-2P 431902-03-3P 431902-04-4P 431902-05-5P
431902-06-6P 431902-07-7P 431902-08-8P 431902-09-9P 438044-29-2P
438044-30-5P 438044-35-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

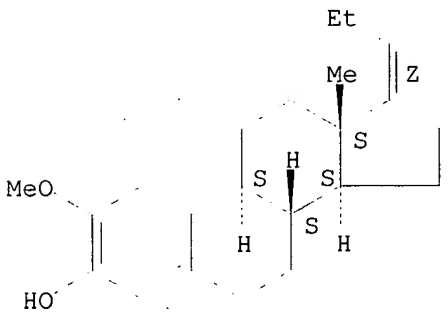
IT 53-16-7, Estrone, reactions 106-95-6, Allyl bromide, reactions
1779-51-7, Butyltriphenylphosphonium bromide 4784-77-4, Crotyl bromide
5815-08-7 6228-47-3, Propyltriphenylphosphonium bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT 26356-54-7P 26357-07-3P 93949-26-9P 431901-79-0P 431901-81-4P
431901-82-5P 431901-83-6P 431901-84-7P 431901-85-8P 431901-89-2P
438044-31-6P 438044-32-7P 438044-33-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT **431901-72-3P 431901-75-6P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

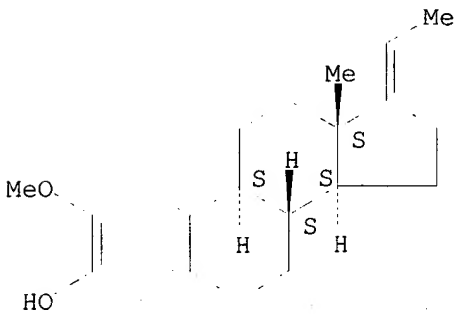
RN 431901-72-3 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 2-methoxy-17-propylidene-, (17Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



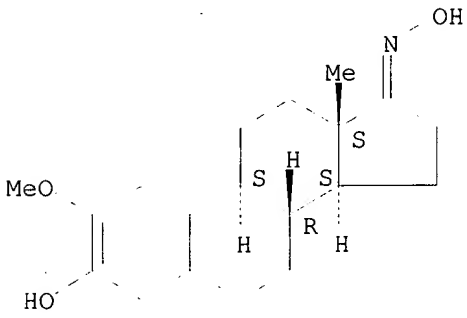
RN 431901-75-6 HCAPLUS
CN 19-Norpregna-1,3,5(10),17(20)-tetraen-3-ol, 2-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



IT **431901-69-8P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)
RN 431901-69-8 HCAPLUS
CN Estra-1,3,5(10)-trien-17-one, 3-hydroxy-2-methoxy-, oxime (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



L41 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 2002:408687 HCAPLUS
DN 137:6309
ED Entered STN: 31 May 2002
TI Preparation of 2-methoxyestradiol analogs as antiangiogenic agents
IN **Agoston, Gregory; Shah, Jamshed H.; Hunsucker, Kimberly A.; Pribluda, Victor; Lavallee, Theresa M. ; Green, Shawn J.; Herbstritt, Christopher J.; Zhan, Xiaoguo H.; Treston, Anthony**
PA **Entremed, Inc., USA**
SO PCT Int. Appl., 86 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07J001-00
CC 32-3 (Steroids)

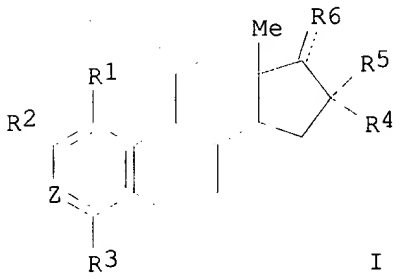
Section cross-reference(s): 1, 2, 63

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002042319	A2	20020530	WO 2001-US26490	20010824
	WO 2002042319	A3	20030313		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2001088386	A5	20020603	AU 2001-88386	20010824
	EP 1343803	A2	20030917	EP 2001-968112	20010824
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
PRAI	US 2000-253385P	P	20001127		
	US 2000-255302P	P	20001213		
	US 2001-278250P	P	20010323		
	US 2001-933894	A	20010821		
	WO 2001-US26490	W	20010824		

OS MARPAT 137:6309

GI



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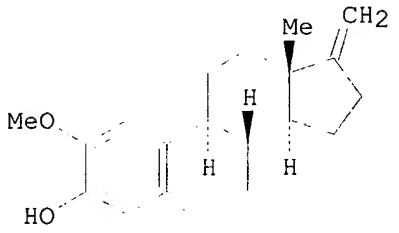


II

AB 2-Methoxyestradiol analogs, such as I [R1, R3 = H, halo, CN, alkyl, OH, CH2OH, NH2, alkylamino; R2 = N3, CN, C.tplbond.CR, C=CHR, C.tplbond.CH, OR, amino; R = H, alkyl; Z = COH, COAc; dashed bond = single bond or double bond; R6 = H, OH, O, oxime, amino, alkyl, alkenyl; R4, R5 = H, alkyl, alkenyl, alkynyl], were prepared for treating mammalian disease characterized by undesirable angiogenesis. Thus, 2-methoxyestradiol analog II was prepared by the reaction of methyltriphenylphosphonium bromide and 2-methoxyestrone. In vitro evaluation against MDA-MB-231 breast tumor cells and HUVEC endothelial cells, II showed IC50 0.24±0 and 0.19±0.19 resp.

ST methoxyestradiol deriv prepn antiangiogenic antitumor; estradiol methoxy deriv prepn antiangiogenic antitumor

IT Cell proliferation
(inhibition; preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT Mammary gland, neoplasm
(inhibitors; preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT Antitumor agents
(mammary gland; preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT Angiogenesis inhibitors

Human
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT Estrogens
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT 53-63-4P, Estra-1,3,5(10)-trien-3-ol **431901-72-3P** 431901-73-4P
431901-75-6P 431901-77-8P 431901-83-6P 431901-89-2P
431901-91-6P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT 1818-12-8P 4953-96-2P 6298-51-7P 6301-87-7P 6599-97-9P
7291-57-8P 10332-20-4P 32162-96-2P 41259-43-2P 94440-60-5P
165619-07-8P 165881-61-8P 192062-02-5P 229486-18-4P 431901-68-7P
431901-69-8P 431901-70-1P 431901-71-2P 431901-74-5P
431901-76-7P 431901-78-9P 431901-82-5P 431901-84-7P 431901-86-9P
431901-87-0P 431901-88-1P 431901-92-7P 431901-93-8P 431901-94-9P
431901-95-0P 431901-96-1P 431901-97-2P 431901-98-3P 431901-99-4P
431902-00-0P 431902-01-1P 431902-02-2P 431902-03-3P 431902-04-4P
431902-05-5P 431902-06-6P 431902-07-7P 431902-08-8P 431902-09-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

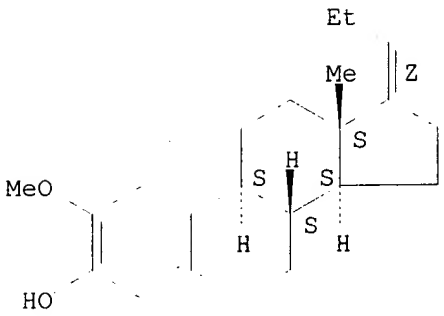
IT 53-16-7, Estrone, reactions 64-18-6, Formic acid, reactions 100-39-0, Benzyl bromide 106-95-6, Allyl bromide, reactions 362-07-2, 2-Methoxyestradiol 1530-32-1, Ethyl triphenylphosphonium bromide 1779-49-3, Methyl triphenylphosphonium bromide 1779-51-7, Butyl triphenylphosphonium bromide 4784-77-4, Crotyl bromide 5815-08-7, tert-Butoxy bis(dimethylamino)methane 6228-47-3, Propyl triphenylphosphonium bromide 17640-15-2, Methyl cyanoformate
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT 26356-54-7P 26357-07-3P 93949-26-9P 431901-79-0P 431901-80-3P
431901-81-4P 431901-85-8P 431901-90-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT **431901-72-3P 431901-75-6P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

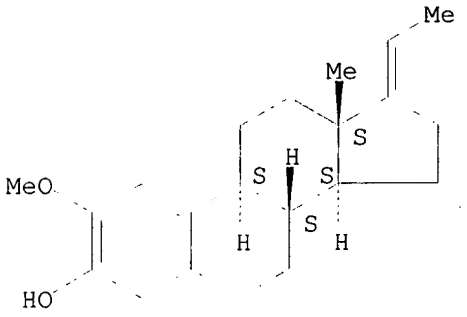
RN 431901-72-3 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 2-methoxy-17-propylidene-, (17Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



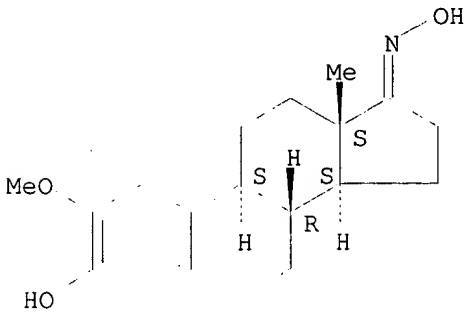
RN 431901-75-6 HCAPLUS
CN 19-Norpregna-1,3,5(10),17(20)-tetraen-3-ol, 2-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



IT **431901-69-8P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)
RN 431901-69-8 HCAPLUS
CN Estra-1,3,5(10)-trien-17-one, 3-hydroxy-2-methoxy-, oxime (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

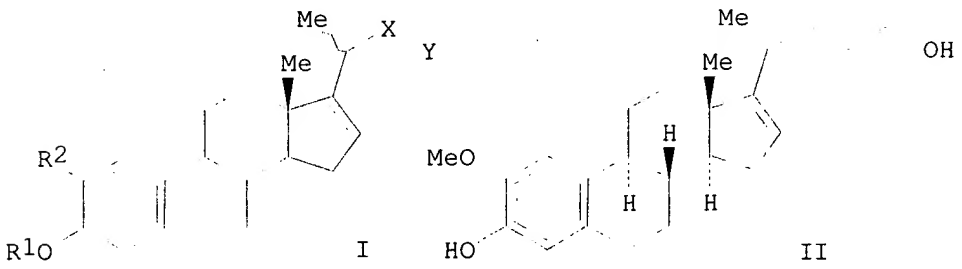


L41 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 2001:833342 HCAPLUS
DN 135:358085

ED Entered STN: 16 Nov 2001
TI Preparation of 2-substituted pregna-1,3,5(10)-triene and chola-1,3,5(10)-triene derivatives with antiproliferative and antiangiogenic activity
IN Hesse, Robert Henry; Setty, Sundara Katugam Srinivasasetty; Pechet, Maurice Murdoch; Gile, Michael
PA Marsden, John Christopher, UK; Research Institute for Medicine and Chemistry Inc.
SO PCT Int. Appl., 40 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07J041-00
ICS A61K031-57; C07J009-00; C07J013-00; C07J051-00; A61K031-575; A61P005-30; A61P035-00
CC 32-5 (Steroids)
Section cross-reference(s): 1, 63
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2001085755	A1	20011115	WO 2001-GB2103	20010511
W: AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1287017	A1	20030305	EP 2001-928120	20010511
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003532737	T2	20031105	JP 2001-582354	20010511
NO 2002005392	A	20030109	NO 2002-5392	20021111
US 2003158167	A1	20030821	US 2003-275257	20030313
PRAI US 2000-203462P	P	20000511		
WO 2001-GB2103	W	20010511		

OS MARPAT 135:358085
GI



AB Compds. of formula I [R1 = H, protecting group; R2 = OH, alkoxy, CHO, alkenyl, etc.; X = alkylene, bond; Y = CHO, (substituted) CH2OH, etc.] are prepared which exhibit potent cell modulating activity, including antiproliferative and antiangiogenic effects. Thus, 2-methoxy-3-triisopropylsilyloxy-19-norpregn-1,3,5(10),17(20)Z-tetraene (preparation given) is reacted with Me acrylate, reduced with LiAlH4, and desilylated with TBAF to give II.
ST pregnatriene deriv prepn antiproliferative antiangiogenic; cholatriene

deriv prepn antiproliferative antiangiogenic; antiproliferative pregnatriene cholatriene deriv; antiangiogenic pregnatriene cholatriene deriv

IT Angiogenesis inhibitors
Antitumor agents
(preparation of 2-substituted pregnatriene and cholatriene derivs. with antiproliferative and antiangiogenic activity)

IT Proliferation inhibition
(proliferation inhibitors; preparation of 2-substituted pregnatriene and cholatriene derivs. with antiproliferative and antiangiogenic activity)

IT 372952-25-5P 372952-27-7P 372952-29-9P 372952-30-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 2-substituted pregnatriene and cholatriene derivs. with antiproliferative and antiangiogenic activity)

IT 372952-23-3P 372952-24-4P 372952-28-8P 372952-31-3P 372952-32-4P
372952-33-5P 372952-34-6P 372952-35-7P 372952-36-8P 372952-37-9P
372952-38-0P 372952-39-1P 372952-40-4P 372952-41-5P 372952-42-6P
372952-43-7P 372952-44-8P 372952-45-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2-substituted pregnatriene and cholatriene derivs. with antiproliferative and antiangiogenic activity)

IT 96-33-3, Methyl acrylate 305812-67-3 372952-58-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 2-substituted pregnatriene and cholatriene derivs. with antiproliferative and antiangiogenic activity)

IT **229486-17-3P** 305812-87-7P 305812-89-9P 305812-91-3P
305812-97-9P 372952-46-0P 372952-47-1P 372952-48-2P 372952-49-3P
372952-50-6P 372952-51-7P 372952-52-8P 372952-53-9P 372952-54-0P
372952-55-1P 372952-56-2P 372952-57-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2-substituted pregnatriene and cholatriene derivs. with antiproliferative and antiangiogenic activity)

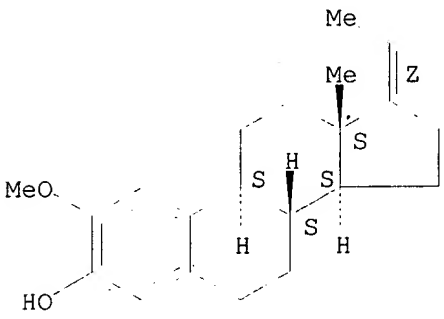
RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Cushman, M; JOURNAL OF MEDICINAL CHEMISTRY 1995, V38(12), P2041 HCAPLUS
(2) Marsden, J; WO 0068246 A 2000 HCAPLUS
(3) Mitsubishi Chemical Industries Co Ltd; JP 54112849 A HCAPLUS
(4) Mitsubishi Chemical Industries Co Ltd; JP 54112850 A HCAPLUS
(5) Mitsubishi Chemical Industries Co Ltd; JP 54117454 A HCAPLUS
(6) Mitsubishi Chemical Industries Co Ltd; JP 54117455 A HCAPLUS
(7) Mitsubishi Chemical Industries Co Ltd; JP 54117456 A HCAPLUS
(8) Mitsubishi Chemical Industries Co Ltd; JP 54112849 A 1979 HCAPLUS
(9) Mitsubishi Chemical Industries Co Ltd; JP 54112850 A 1979 HCAPLUS
(10) Mitsubishi Chemical Industries Co Ltd; JP 54117454 A 1979 HCAPLUS
(11) Mitsubishi Chemical Industries Co Ltd; JP 54117455 A 1979 HCAPLUS
(12) Mitsubishi Chemical Industries Co Ltd; JP 54117456 A 1979 HCAPLUS
(13) Mitsubishi Chemical Industries Co Ltd; PATENT ABSTRACTS OF JAPAN 1979, V003(133), PC-063
(14) Mitsubishi Chemical Industries Co Ltd; PATENT ABSTRACTS OF JAPAN 1979, V003(133), PC-063
(15) Ruggieri, P; US 3562260 A 1971 HCAPLUS

IT **229486-17-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2-substituted pregnatriene and cholatriene derivs. with antiproliferative and antiangiogenic activity)

RN 229486-17-3 HCAPLUS

CN 19-Norpregna-1,3,5(10),17(20)-tetraen-3-ol, 2-methoxy-, (17Z)- (9CI) (CA INDEX NAME)

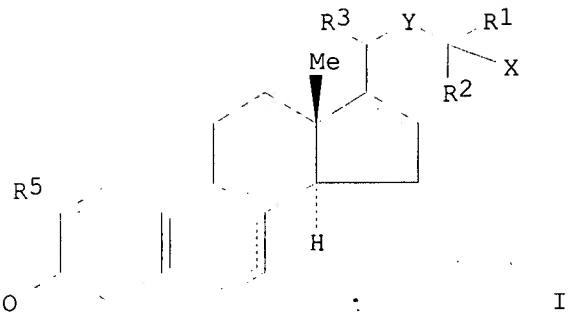
Absolute stereochemistry.
Double bond geometry as shown.



L41 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 2000:814500 HCAPLUS
DN 133:350395
ED Entered STN: 21 Nov 2000
TI Synthesis of cholestane compounds with a c17-alkyl side chain and an aromatic A-ring for use in cell modulating therapy
IN Hesse, Robert Henry; Setty, Sundara Katugam Srinivasasetty; Ramgopal, Malathi; Kugabalusooriar, Sanga
PA Marsden, John, Christopher, UK; Research Institute for Medicine and Chemistry Inc.
SO PCT Int. Appl., 75 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07J009-00
ICS C07J041-00; A61K031-575; C07J051-00; A61P017-02; A61P019-08; A61P037-06; A61P029-00; A61P035-00; A61P021-00; A61P009-10; A61P005-20; A61P017-00; A61P009-12; A61P019-02; A61P011-06; A61P025-28; A61P015-18; A61P007-02; A61P003-06
CC 32-7 (Steroids)
Section cross-reference(s): 1, 2
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000068246	A1	20001116	WO 2000-GB1813	20000511
	W: AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1179005	A1	20020213	EP 2000-927569	20000511
	EP 1179005	B1	20031119		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	ZA 2001009272	A	20021128	ZA 2001-9272	20011109
	NO 2001005520	A	20020109	NO 2001-5520	20011112
PRAI	GB 1999-10934	A	19990511		
	WO 2000-GB1813	W	20000511		

OS MARPAT 133:350395
GI



I

AB Synthesis of cholestane compds. (I) [R1 and R2, which may be the same or different, = alkyl, alkenyl, alkynyl; R3 = Me having α- or β-configuration; R4 = H or an etherifying or esterifying group; R5 = H, OH, alkoxy; X = OR4, wherein R4 is as defined above, or NR6R7 wherein R6 = H, aliphatic or araliph. organic group, acyl group comprising aliphatic, araliph. or aryl organic group linked to the nitrogen atom by way of a carbonyl group; R7 = H, alkyl; Y = (un)substituted alkylene, alkenylene, alkynylene; dotted lines signify that double bonds may be present at the 16(17)-position and/or either at the 6(7)- and 8(9)-positions or at the 7(8)-position] is disclosed for modulation of cell growth and differentiation, while having low calcemic activity. Thus, I [R1,R2 = Me; R3 = α-Me; R4,R5 = H; X = NHAc; Y = (CH2)4; Δ16 double bond] is prepared by reaction of 3-triisopropylsilyloxy-19-norchol-1,3,5(10),16-tetraene-24-bromide with acetoniltrile followed by reduction of nitrile to amine, methylation of amine with Me lithium, acetylation of the amino with acetic anhydride and desilylation with TBAF.

ST cholestane analog prepn cell growth modulation differentiation; low calcemic activity cholestane analog

IT Steroids, preparation
Steroids, preparation
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(aromatic; synthesis of cholestane compds. with a c17-alkyl side chain and an aromatic A-ring for use in cell modulating therapy)

IT Transplant and Transplantation
(host-vs.-graft reaction; synthesis of cholestane compds. with a c17-alkyl side chain and an aromatic A-ring for use in cell modulating therapy)

IT Arthritis
(psoriatic arthritis; synthesis of cholestane compds. with a c17-alkyl side chain and an aromatic A-ring for use in cell modulating therapy)

IT Hyperparathyroidism
(secondary; synthesis of cholestane compds. with a c17-alkyl side chain and an aromatic A-ring for use in cell modulating therapy)

IT Mental disorder
(senile psychosis; synthesis of cholestane compds. with a c17-alkyl side chain and an aromatic A-ring for use in cell modulating therapy)

IT Heart, disease
(spondylitic; synthesis of cholestane compds. with a c17-alkyl side chain and an aromatic A-ring for use in cell modulating therapy)

IT Aromatic hydrocarbons, preparation
Aromatic hydrocarbons, preparation
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

BIOL (Biological study); PREP (Preparation); USES (Uses)
(steroids; synthesis of cholestane compds. with a c17-alkyl side chain and an aromatic A-ring for use in cell modulating therapy)

IT Anti-inflammatory agents
Antitumor agents
Asthma
Autoimmune disease
Blood coagulation
Bone, disease
Burn
Fertility
Hyperplasia
Hypertension
Intestine, disease
Muscle, disease
Rheumatoid arthritis
Skin, disease
Transplant rejection
Wound healing
(synthesis of cholestane compds. with a c17-alkyl side chain and an aromatic A-ring for use in cell modulating therapy)

IT 57-88-5, Cholest-5-en-3-ol (3β)-, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(blood reduction; synthesis of cholestane compds. with a c17-alkyl side chain and an aromatic A-ring for use in cell modulating therapy)

IT 9002-64-6, Parathyroid hormone
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(suppression; synthesis of cholestane compds. with a c17-alkyl side chain and an aromatic A-ring for use in cell modulating therapy)

IT 305812-17-3P 305812-18-4P 305812-52-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(synthesis of cholestane compds. with a c17-alkyl side chain and an aromatic A-ring for use in cell modulating therapy)

IT 305812-19-5P 305812-20-8P 305812-21-9P 305812-22-0P 305812-23-1P
305812-24-2P 305812-25-3P 305812-26-4P 305812-27-5P 305812-28-6P
305812-29-7P 305812-30-0P 305812-31-1P 305812-32-2P 305812-33-3P
305812-34-4P 305812-35-5P 305812-36-6P 305812-37-7P 305812-38-8P
305812-39-9P 305812-40-2P 305812-41-3P 305812-42-4P 305812-43-5P
305812-44-6P 305812-45-7P 305812-46-8P 305812-47-9P 305812-48-0P
305812-49-1P 305812-50-4P 305812-51-5P 305812-53-7P 305812-54-8P
305812-55-9P 305812-56-0P 305812-57-1P 305812-58-2P 305812-59-3P
305812-60-6P 305812-61-7P 305812-62-8P 305812-63-9P 305812-64-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of cholestane compds. with a c17-alkyl side chain and an aromatic A-ring for use in cell modulating therapy)

IT 74-88-4, Methyl iodide, reactions 75-03-6, Ethyl iodide 75-05-8, Acetonitrile, reactions 78-77-3, Isobutyl bromide 96-33-3 98-88-4, Benzoyl chloride 103-80-0, Phenylacetyl chloride 106-96-7, Propargyl bromide 474-87-3 517-09-9 867-13-0 922-67-8, Methyl propiolate 1439-36-7, 1-Triphenylphosphoranylidene-2-propanone 3234-64-8, 1,1-Diethylpropargylamine 4736-60-1, Ethyl triphenylphosphonium iodide 7103-48-2, Estrone-3-tetrahydropyranyl ether 17963-41-6 305812-65-1 305812-66-2 305812-67-3 305812-69-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of cholestane compds. with a c17-alkyl side chain and an aromatic A-ring for use in cell modulating therapy)

IT **229486-17-3P** 305812-70-8P 305812-71-9P 305812-72-0P
305812-73-1P 305812-75-3P 305812-76-4P 305812-77-5P 305812-79-7P

provided by InfoChem.

STRUCTURE FILE UPDATES: 19 DEC 2003 HIGHEST RN 628722-21-4
DICTIONARY FILE UPDATES: 19 DEC 2003 HIGHEST RN 628722-21-4

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

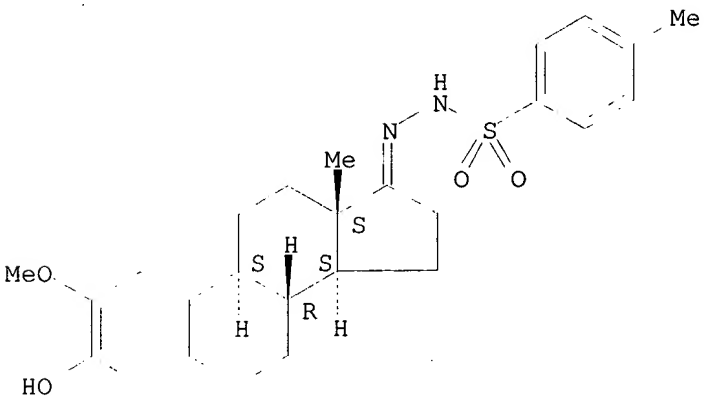
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> d ide can tot l76

L76 ANSWER 1 OF 12 REGISTRY COPYRIGHT 2003 ACS on STN
RN **438044-29-2** REGISTRY
CN Benzenesulfonic acid, 4-methyl-, (3-hydroxy-2-methoxyestra-1,3,5(10)-trien-17-ylidene)hydrazide (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C26 H32 N2 O4 S**
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.
Double bond geometry unknown.



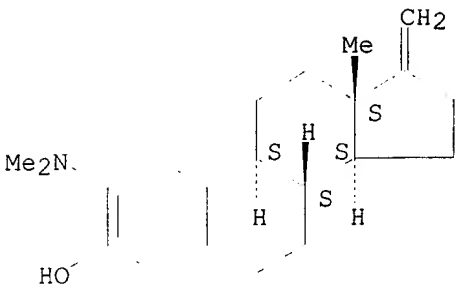
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:47357

L76 ANSWER 2 OF 12 REGISTRY COPYRIGHT 2003 ACS on STN
RN **431901-97-2** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 2-(dimethylamino)-17-methylene-, hydrochloride (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C21 H29 N O . Cl H**
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



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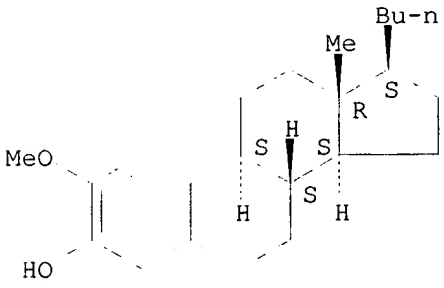
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:47357

REFERENCE 2: 137:6309

L76 ANSWER 3 OF 12 REGISTRY COPYRIGHT 2003 ACS on STN
RN **431901-78-9** REGISTRY
CN 19,21-Dinorchola-1,3,5(10)-trien-3-ol, 2-methoxy- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C23 H34 O2**
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



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3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:224972

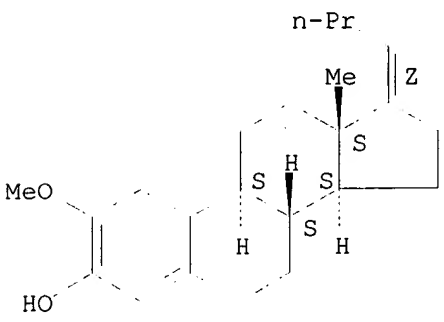
REFERENCE 2: 137:47357

REFERENCE 3: 137:6309

L76 ANSWER 4 OF 12 REGISTRY COPYRIGHT 2003 ACS on STN
RN **431901-77-8** REGISTRY
CN 19,21-Dinorchola-1,3,5(10),17(20)-tetraen-3-ol, 2-methoxy-, (17Z)- (9CI)

(CA INDEX NAME)
FS STEREOSEARCH
MF **C23 H32 O2**
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

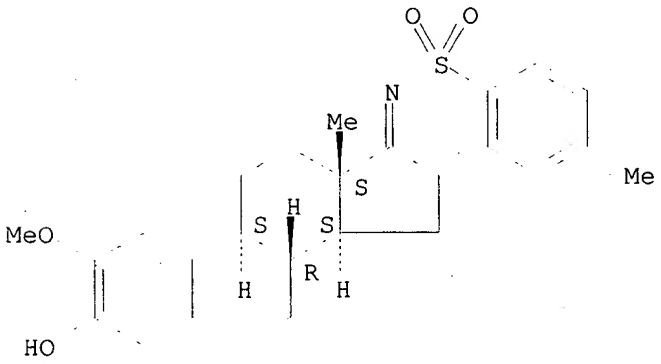
REFERENCE 1: 139:224972

REFERENCE 2: 137:47357

REFERENCE 3: 137:6309

L76 ANSWER 5 OF 12 REGISTRY COPYRIGHT 2003 ACS on STN
RN **431901-76-7** REGISTRY
CN Benzenesulfonamide, N-(3-hydroxy-2-methoxyestra-1,3,5(10)-trien-17-ylidene)-4-methyl- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C26 H31 N O4 S**
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.
Double bond geometry unknown.



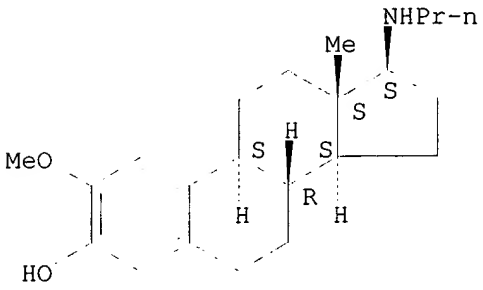
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:6309

L76 ANSWER 6 OF 12 REGISTRY COPYRIGHT 2003 ACS on STN
RN **431901-74-5** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 2-methoxy-17-(propylamino)-, (17β)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C22 H33 N O2**
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

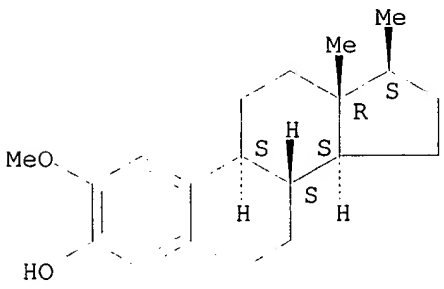
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:47357

REFERENCE 2: 137:6309

L76 ANSWER 7 OF 12 REGISTRY COPYRIGHT 2003 ACS on STN
RN **431901-71-2** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 2-methoxy-17-methyl-, (17β)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C20 H28 O2**
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

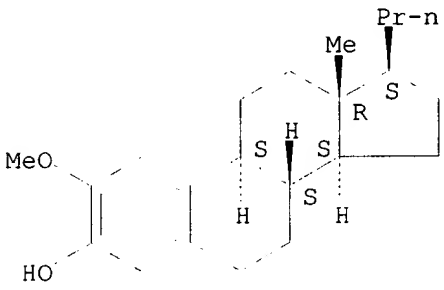
REFERENCE 1: 139:224972

REFERENCE 2: 137:47357

REFERENCE 3: 137:6309

L76 ANSWER 8 OF 12 REGISTRY COPYRIGHT 2003 ACS on STN
RN **431901-70-1** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 2-methoxy-17-propyl-, (17β)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C22 H32 O2**
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

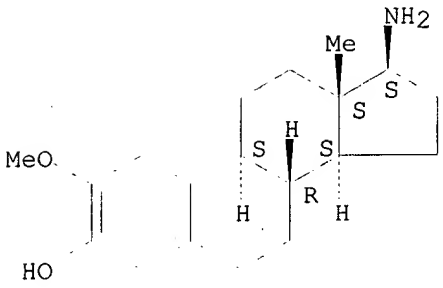
REFERENCE 1: 139:224972

REFERENCE 2: 137:47357

REFERENCE 3: 137:6309

L76 ANSWER 9 OF 12 REGISTRY COPYRIGHT 2003 ACS on STN
RN **431901-68-7** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-amino-2-methoxy-, (17β)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C19 H27 N O2**
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

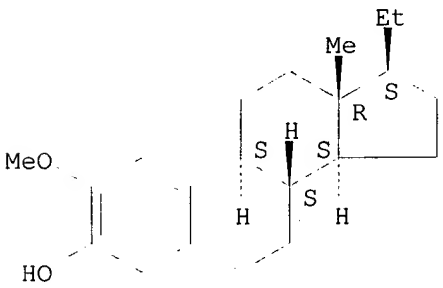
REFERENCE 1: 139:224972

REFERENCE 2: 137:47357

REFERENCE 3: 137:6309

L76 ANSWER 10 OF 12 REGISTRY COPYRIGHT 2003 ACS on STN
RN **229486-18-4** REGISTRY
CN 19-Norpregna-1,3,5(10)-trien-3-ol, 2-methoxy- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C21 H30 O2**
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:224972

REFERENCE 2: 137:47357

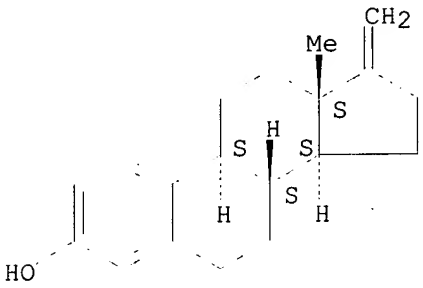
REFERENCE 3: 137:6309

REFERENCE 4: 131:88083

L76 ANSWER 11 OF 12 REGISTRY COPYRIGHT 2003 ACS on STN
RN **34111-53-0** REGISTRY

CN Estra-1,3,5(10)-trien-3-ol, 17-methylene- (7CI, 8CI, 9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C19 H24 O**
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

19 REFERENCES IN FILE CA (1907 TO DATE)
19 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 139:224972

REFERENCE 2: 138:348841

REFERENCE 3: 136:37829

REFERENCE 4: 133:208036

REFERENCE 5: 132:347795

REFERENCE 6: 132:308544

REFERENCE 7: 129:54482

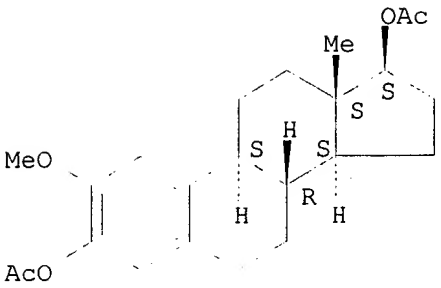
REFERENCE 8: 128:294938

REFERENCE 9: 128:154277

REFERENCE 10: 127:293468

L76 ANSWER 12 OF 12 REGISTRY COPYRIGHT 2003 ACS on STN
RN **7291-57-8** REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-, diacetate, (17β)- (9CI)
(CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Estra-1,3,5(10)-triene-3,17β-diol, 2-methoxy-, diacetate (7CI, 8CI)
CN Estradiol, 2-methoxy-, diacetate (6CI)
FS STEREOSEARCH
MF **C23 H30 O5**
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

11 REFERENCES IN FILE CA (1907 TO DATE)
11 REFERENCES IN FILE CAPLUS (1907 TO DATE)
3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 139:369731

REFERENCE 2: 139:224972

REFERENCE 3: 137:47357

REFERENCE 4: 137:6309

REFERENCE 5: 134:295993

REFERENCE 6: 117:226505

REFERENCE 7: 90:121859

REFERENCE 8: 73:116788

REFERENCE 9: 72:121765

REFERENCE 10: 64:53436

=> d his l76-

(FILE 'REGISTRY' ENTERED AT 10:00:20 ON 21 DEC 2003)
L76 12 S L73,L75

FILE 'HCAOLD' ENTERED AT 10:10:31 ON 21 DEC 2003
L77 4 S L76

FILE 'HCAPLUS' ENTERED AT 10:10:45 ON 21 DEC 2003
L78 30 S L76
L79 27 S L78 AND (PD<=20010208 OR PRD<=20010208 OR AD<=20010208)
L80 3 S L78 AND L47-L60
L81 29 S L63,L79-L80
L82 2 S L78 NOT L81

FILE 'HCAOLD' ENTERED AT 10:12:46 ON 21 DEC 2003
SEL AN L77
EDIT /AN /OREF

FILE 'HCAPLUS' ENTERED AT 10:13:12 ON 21 DEC 2003
L83 6 S E66-E69
L84 5 S L83 NOT MAZUR ?/AU

L85 31 S L81,L84
L86 26 S L81 NOT L84

FILE 'REGISTRY' ENTERED AT 10:14:28 ON 21 DEC 2003

=> fil hcaold
FILE 'HCAOLD' ENTERED AT 10:14:44 ON 21 DEC 2003

PRE-1967 CHEMICAL ABSTRACTS FILE WITH HOUR-BASED PRICING
FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

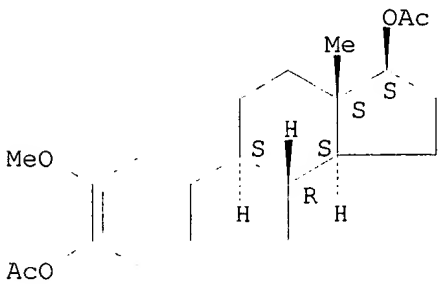
This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> d l77 all hitstr tot

L77 ANSWER 1 OF 4 HCAOLD COPYRIGHT 2003 ACS on STN
AN CA64:10030d CAOLD
TI thin-layer chromatography of estrogens on Kieselgel G
AU Lisboa, Belisario P.
IT 53-63-4 362-05-0 362-07-2 362-08-3 472-56-0 472-57-1
474-86-2 482-49-5 517-09-9 566-75-6 570-30-9 571-92-6
793-89-5 901-93-9 1035-77-4 1089-80-1 1150-90-9 1228-72-4
1228-73-5 1232-80-0 1247-70-7 1247-71-8 1474-52-8 1474-53-9
1476-34-2 1971-65-9 2208-12-0 2284-32-4 2464-15-5 3398-11-6
3434-79-5 3434-88-6 3563-27-7 3583-03-7 4551-97-7 5444-22-4
5976-62-5 6030-91-7 7004-98-0 7291-41-0 7291-47-6 7291-49-8
7291-51-2 7291-52-3 7291-53-4 7291-54-5 7291-56-7
7291-57-8 7323-86-6 7323-87-7 7323-90-2 7323-91-3
7323-92-4 7533-97-3 7684-84-6
IT **7291-57-8**
RN 7291-57-8 HCAOLD
CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-, diacetate, (17β)- (9CI) (CA INDEX NAME)

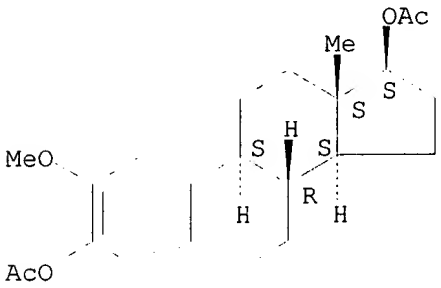
Absolute stereochemistry.



L77 ANSWER 2 OF 4 HCAOLD COPYRIGHT 2003 ACS on STN

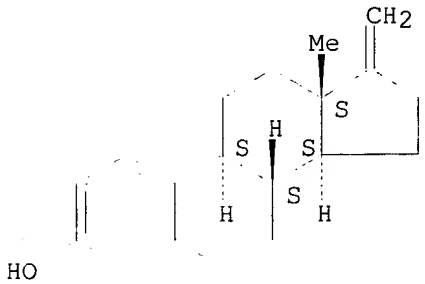
AN CA61:8583b CAOLD
TI use of double derivs. in the gas chromatography in urinary estrogens
AU Cox, R. I.; Bedford, A. R.
IT 2394-15-2 3434-85-3 5976-55-6 **7291-57-8** 18880-67-6
18880-86-9
IT **7291-57-8**
RN 7291-57-8 HCAOLD
CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-, diacetate, (17β)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



L77 ANSWER 3 OF 4 HCAOLD COPYRIGHT 2003 ACS on STN
AN CA56:515f CAOLD
TI distance effects in the steroid series - (II) influence of 17-substituents
on pK values of steroidal phenols
AU Legrand, Maurice; Delaroff, V.; Mathieu, J.
TI vegetable steroids-their utilization in the hemisynthesis of sexual
hormones and suprarenals
AU Grigot, Pierre
IT 53-63-4 1667-98-7 **34111-53-0** 35451-11-7 108041-85-6
IT **34111-53-0**
RN 34111-53-0 HCAOLD
CN Estra-1,3,5(10)-trien-3-ol, 17-methylene- (7CI, 8CI, 9CI) (CA INDEX NAME)

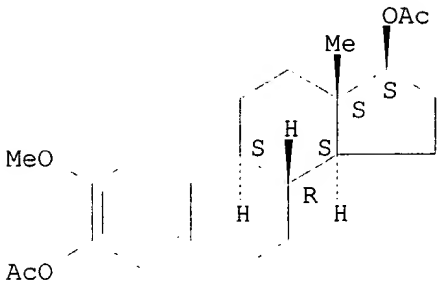
Absolute stereochemistry.



L77 ANSWER 4 OF 4 HCAOLD COPYRIGHT 2003 ACS on STN
AN CA52:13765i CAOLD
TI synthesis of 2-methoxyestrogens
AU Fishman, Jack
IT 362-07-2 362-08-3 **7291-57-8** 38781-50-9 52717-98-3
65932-49-2 65932-50-5 65932-51-6 65932-52-7 65932-53-8 84509-93-3
103278-44-0 120024-00-2
IT **7291-57-8**
RN 7291-57-8 HCAOLD
CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-, diacetate, (17β)- (9CI)

(CA INDEX NAME)

Absolute stereochemistry.



=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 10:14:51 ON 21 DEC 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 21 Dec 2003 VOL 139 ISS 26
FILE LAST UPDATED: 19 Dec 2003 (20031219/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> => => d all hitstr tot l88

L88 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 1966:53436 HCAPLUS
DN 64:53436
OREF 64:**10030c-d**
ED Entered STN: 22 Apr 2001
TI Thin-layer chromatography of estrogens on Kieselgel G.
AU Lisboa, B. P.
CS Karolinska Sjukhuset, Stockholm
SO Clinica Chimica Acta (1966), 13(2), 179-99
CODEN: CCATAR; ISSN: 0009-8981
DT Journal
LA German
CC 58 (Hormones)
AB A method for the separation and characterization of 51 steroid estrogens by ascending chromatography on silica gel G after single and multiple chromatography is presented. The steroids are characterized by their Rf-values in several systems, color reactions, and derivative formation. The possibility of separating steroids of similar polarity by thin-layer chromatography is discussed here, and compared with the results obtained

by other anal. procedures. Also, the correlation between steroid structure and mobility is discussed.

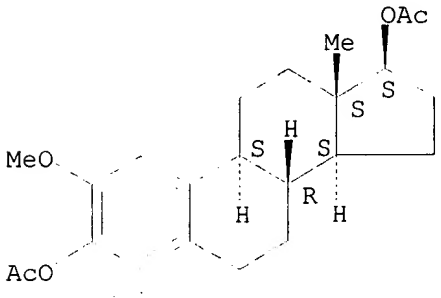
IT Estrogenic hormones or principles
(chromatography of)

IT 16,17-Secoestra-1,3,5(10)-trien-17-oic acid, 3β-hydroxy-
Estra-1,3,5(10)-triene-16α,17β-diol, 3-methexy-
Estra-1,3,5(10-trien-17-one, 3,15α-dihydoxy-
Estra-1,3,6(10)-triene-3,16α,17β-triol, 2-methoxy-
(chromatography of)

IT 50-27-1, Estriol 50-28-2, Estradiol 53-16-7, Estrone 53-63-4, Estra-1,3,5(10)-trien-3-ol 57-91-0, 17α-Estradiol 362-05-0, Estra-1,3,5(10)-triene-2,3,17β-triol 362-08-3, Estra-1,3,5(10-trien-17-one, 3-hydroxy-2-methoxy- 472-56-0, Estra-1,3,5(10)-trien-3-ol, 16α,17α-epoxy- 472-57-1, Estra-1,3,5(10)-trien-3-ol, 16β,17β-epoxy- 474-86-2, Equilin 482-49-5, Doisynolic acid 517-09-9, Equilenin 547-81-9, Estra-1,3,5(10)-triene-3,16β,17β-triol 566-75-6, Estra-1,3,5(10)-trien-16-one, 3,17β-dihydroxy- 566-76-7, Estra-1,3,5(10-trien-17-one, 3,16α-dihydroxy- 570-30-9, Estra-1,3,5(10)-triene-3,15α,17β-triol 571-92-6, Estra-1,3,5(10)-trien-6-one, 3,17β-dihydroxy- 793-89-5, Estra-1,3,5(10)-triene-3,16β,17α-triol 901-93-9, Estrone, acetate 966-06-3, Estra-1,3,5(10-trien-17-one, 3,16β-dihydroxy- 1035-77-4, Estra-1,3,5(10)-trien-17β-ol, 3-methoxy- 1089-80-1, Estra-1,3,5(10),9(11)-tetraen-17-one, 3-hydroxy- 1150-90-9, Estra-1,3,5(10),16-tetraen-3-ol 1228-72-4, Estra-1,3,5(10)-triene-3,16α,17α-triol 1228-73-5, Estra-1,3,5(10)-triene-16,17-dione, 3-hydroxy- 1229-24-9, Estra-1,3,5(10)-triene-3,6α,17β-triol 1229-25-0, Estra-1,3,5(10-trien-17-one, 3,6β-dihydroxy- 1232-80-0, Estra-1,3,5(10)-triene-2,3,16α,17β-tetrol 1247-70-7, Estra-1,3,5(10-trien-17-one, 3,16β-dihydroxy-, diacetate 1247-71-8, Estra-1,3,5(10-trien-17-one, 3,16α-dihydroxy-, diacetate 1474-52-8, 17α-Estradiol, diacetate 1476-78-4, Estra-1,3,5(10-trien-17-one, 3,6α-dihydroxy- 1971-65-9, Estra-1,3,5(10),6-tetraene-3,17β-diol, diacetate 2208-12-0, Estra-1,3,5(10),6-tetraen-17-one, 3-hydroxy- 2284-32-4, Estriol, triacetate 2487-47-0, Estra-1,3,5(10-trien-17-one, 3,7β-dihydroxy- 2487-49-2, Estra-1,3,5(10-trien-17-one, 3,7α-dihydroxy- 3131-23-5, Estra-1,3,5(10-trien-17-one, 3,4-dihydroxy- 3398-11-6, Estra-1,3,5(10)-triene-3,7α,17β-triol 3434-79-5, Estra-1,3,5(10)-triene-16β,17β-diol, 3-methoxy- 3434-88-6, Estradiol, diacetate 3563-27-7, Estra-1,3,5(10),7-tetraene-3,17β-diol 3583-03-7, Estra-1,3,5(10)-triene-3,6β,17β-triol 4551-97-7, Estra-1,3,5(10)-triene-6β,17β-diol, 3-methoxy- 5210-15-1, Estra-1,3,5(10-trien-17-one, 3,11α-dihydroxy- 5444-22-4, Estra-1,3,5(10)-triene-3,11β,17β-triol 5976-62-5, Estra-1,3,5(10-trien-17-one, 4-hydroxy-3-methoxy- 6030-91-7, Equilenin, acetate 6803-21-0, Estra-1,3,5(10-trien-17-one, 3,11β-dihydroxy- 7004-98-0, Estra-1,3,5(10)-triene-16α,17α-diol, 3-methoxy- 7291-41-0, Estra-1,3,5(10),6-tetraene-3,17β-diol 7291-47-6, Estra-1,3,5(10)-triene-6α,17β-diol, 3-methoxy- 7291-49-8, Estra-1,3,5(10)-triene-3,6α,16α,17β-tetrol 7291-51-2, Estra-1,3,5(10),6-tetraen-3-ol, acetate 7291-52-3, Estra-1,3,5(10),9(11)-tetraen-17-one, 3-hydroxy-, acetate 7291-53-4, Estra-1,3,5(10)-triene-11,17-dione, 3-hydroxy-, acetate 7291-54-5, Estra-1,3,5(10)-triene-16,17-dione, 3-hydroxy-, acetate 7291-56-7, Estra-1,3,5(10)-triene-2,3,17β-triol, triacetate **7291-57-8**, Estra-1,3,5(10)-triene-3,17β-diol, 2-methoxy-, diacetate 7323-86-6, Estra-1,3,5(10)-trien-6-one, 3,16α,17β-trihydroxy- 7323-87-7, Estra-1,3,5(10)-triene-3,6,7,17β-tetrol 7323-90-2, Estra-1,3,5(10-trien-17-one, 3,6β-dihydroxy-, diacetate 7323-91-3, Estra-1,3,5(10)-triene-3,17β-diol, 6β,7β-epoxy-, diacetate 7323-92-4, Estra-1,3,5(10)-triene-3,6α,7β,17β-tetrol, tetraacetate 7533-97-3, Estra-1,3,5(10)-triene-11,17-dione, 3-hydroxy- 7684-84-6,

Estra-1,3,5(10)-triene-7,17-dione, 3-hydroxy-, acetate 109784-48-7,
2-Phenanthrenecarboxylic acid, 1-ethyl-1,2,3,4,4a,9,10,10a-octahydro-7-hydroxy-2-methyl-
(chromatography of)
IT 362-07-2, Estra-1,3,5(10)-triene-3,17β-diol, 2-methoxy- 1476-34-2,
Estra-1,3,5(10)-triene-6,17-dione, 3-hydroxy- 2464-15-5,
Estra-1,3,5(10)-triene-7,17-dione, 3-hydroxy- 3398-12-7,
Estra-1,3,5(10)-trien-7-one, 3,17β-dihydroxy-
(preparation of)
IT **7291-57-8**, Estra-1,3,5(10)-triene-3,17β-diol, 2-methoxy-, diacetate
(chromatography of)
RN 7291-57-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-, diacetate, (17β)- (9CI) (CA INDEX NAME)

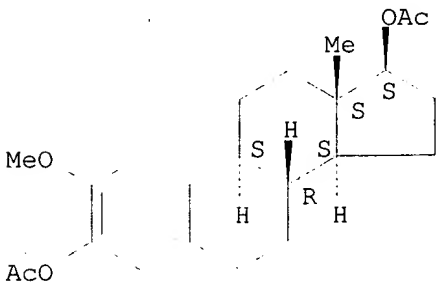
Absolute stereochemistry.



L88 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 1964:449185 HCAPLUS
DN 61:49185
OREF 61:**8583a-c**
ED Entered STN: 22 Apr 2001
TI The use of double derivatives in the gas chromatography of urinary estrogens
AU Cox, R. I.; Bedford, A. R.
CS Univ. Adelaide
SO Steroids (1964), 3(6), 663-9
CODEN: STEDAM; ISSN: 0039-128X
DT Journal
LA Unavailable
CC 58 (Hormones)
AB Double derivs. of urinary estrogens, either 3-Me ether acetates or 3-Me ether trimethylsilyl ethers, were prepd, and suitable conditions for their chromatography investigated. Second- and 3rd-trimester pregnancy urine exts. showed well defined sym. peaks at characteristic retention times for derivs. of the 3 major estrogens (estrone, estradiol, and estriol) on the gas chromatograph recordings. Background interference was more evident in the 1st-trimester pregnancy urine but recordings were satisfactory where concns. of 30-50 γ/24 hrs. were present. Since double derivs. may be prepared as readily as single ones, the extra chemical purification obtained in their preparation before gas chromatography is an advantage in detection and estimation of these compds. in biol. samples.
IT Urine
(analysis, separation of estrogens)
IT Estra-1,3,5(10)-triene, 3-methoxy-16α,17β-bis(trimethylsiloxy)-
Estra-1,3,5(10)-triene, 3-methoxy-17β-(trimethylsiloxy)-
Estra-1,3,5(10)-triene-16α,17β-diol, 3-methexy-, diacetate
(gas chromatography of)
IT 18880-67-6, Silane, [(3-methoxyestra-1,3,5(10)-trien-17β-

yl)oxy]trimethyl- 18880-86-9, Silane, [(3-methoxyestra-1,3,5(10)-trien-16α,17β-ylene)dioxy]bis[trimethyl-
(chromatography (gas) of)
IT 53-06-5, Cortisone 1624-62-0, Estra-1,3,5(10-trien-17-one, 3-methoxy- 5976-55-6, Estra-1,3,5(10)-trien-17β-ol, 3-methoxy-, acetate **7291-57-8**, Estra-1,3,5(10)-triene-3,17β-diol, 2-methoxy-, diacetate
(chromatography of)
IT **7291-57-8**, Estra-1,3,5(10)-triene-3,17β-diol, 2-methoxy-, diacetate
(chromatography of)
RN 7291-57-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-, diacetate, (17β)- (9CI) (CA INDEX NAME)

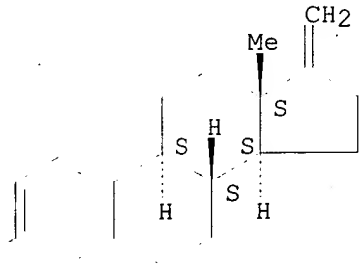
Absolute stereochemistry.



L88 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 1962:2540 HCAPLUS
DN 56:2540
OREF 56:**515f-g**
ED Entered STN: 22 Apr 2001
TI Distance effects in the steroid series. II. Influence of 17-substituents on pK values of steroidal phenols
AU Legrand, Maurice; Delaroff, Vladimir; Mathieu, Jean
CS Roussel Uclaf, Paris
SO Bulletin de la Societe Chimique de France (1961) 1346-8
CODEN: BSCFAS; ISSN: 0037-8968
DT Journal
LA Unavailable
CC 36 (Steroids)
AB The pK values for steroidal phenols were found to vary with the type of substitution in the D-ring. Measurements were made spectrophotometrically in MeOH-MeONa and Na2B4O7.10H2O-Na2CO3 solns. at concns. of 2 + 10-4M and the values reported as pK-pK 17β-estradiol as follows: estra-1,3,5(10)-trien-3-ol (-0.01, 0.00); 17α-estradiol (-0.03, 0.00); D-homo-17aβ-estradiol (0.00, 0.01); 17-methyleneestra-1,3,5(10)-trien-3-ol (-0.02, -0.05); 17β-acetylestra-1,3,5(10)-trien-3-ol (- 0.07, - 0.06); D-homoestrone (-0.09, -0.10); estrone (-0.10, -0.10). The small differences were found to be statistically significant.
IT Steroids
(distant group effect on)
IT Steroids
(natural sources of)
IT Substituents
(neighboring, ionization (pK) of steroidal phenols in relation to)
IT Ionization
(of steroidal phenols, neighboring group effect on)
IT D-Homoestra-1,3,5(10)-trien-17-one, 3-hydroxy-
(ionization of)

IT 53-16-7, Estrone 53-63-4, Estra-1,3,5(10)-trien-3-ol 57-91-0, 17α-Estradiol 1667-98-7, 19-Norpregna-1,3,5(10)-trien-20-one, 3-hydroxy- **34111-53-0**, Estra-1,3,5(10)-trien-3-ol, 17-methylene- 35451-11-7, D-Homoestra-1,3,5(10)-triene-3,17β-diol
(ionization of)
IT **34111-53-0**, Estra-1,3,5(10)-trien-3-ol, 17-methylene-
(ionization of)
RN 34111-53-0 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methylene- (7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



L88 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 1962:2539 HCAPLUS
DN 56:2539
OREF 56:**515f**
ED Entered STN: 22 Apr 2001
TI Vegetable steroids. Their utilization in the hemisynthesis of sexual hormones and suprarenals
AU Grigot, Pierre
SO Prods. Pharm. (1961), 16, 379-401
DT Journal
LA Unavailable
CC 36 (Steroids)
AB A review with 78 references.
IT Steroids
(distant group effect on)
IT Steroids
(natural sources of)

L88 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 1958:77293 HCAPLUS
DN 52:77293
OREF 52:**13765i,13766a-h**
ED Entered STN: 22 Apr 2001
TI Synthesis of 2-methoxyestrogens
AU Fishman, Jack
CS Sloan-Kettering Inst. for Cancer Research, New York, NY
SO Journal of the American Chemical Society (1958), 80, 1213-16
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA Unavailable
CC 10 (Organic Chemistry)
OS CASREACT 52:77293
AB Estrone (I) (1.71 g.) added to 0.210 g. KOH in 50 cc. absolute EtOH, warmed, treated with 0.853 g. 2,5-Cl(O2N)C6H3Bz (II), refluxed 24 hrs., concentrated to half the original volume, cooled, poured into N NaOH, extracted with CHCl3, and the extract evaporated yielded 1.365 g. 3-(2-benzoyl-4-nitrophenyl) ether (III) of I, m. 240-3° (MeOH), [α]26D 88°; the aqueous alkaline solution acidified gave 0.7 g. unchanged I. III (100 mg.) in 0.5 cc. cold. concentrated

H2SO4 treated after 0.5 hr. with 4 cc. glacial AcOH then with 0.5 cc. 30% H2O2, allowed to stand 0.5 hr., poured into iced H2O, filtered, the solid washed with H2O, treated with excess CH2N2 in Et2O, the resulting needles, m. 144-7°, refluxed 1 hr. with piperidine, diluted with C6H6, washed with dilute H2SO4, the C6H6 layer extracted with dilute aqueous NaOH, and the aqueous extract acidified and extracted with CHCl3 gave a few crystals of the 13,17-secolactone, m. 204-7°. 17β-Estradiol (IV) (5 g.) and 0.586 g. KOH in 100 cc. EtOH refluxed 48 hrs. with 2.4 g. II, concentrated to half the original volume, poured into 200 cc. N NaOH, extracted with CHCl3, the extract dried, evaporated, and the residual viscous oil dissolved in 50 cc. 1:1 petr. ether-C6H6 and chromatographed on 150 g. Al2O3 gave 90 mg. II, m. 114-16°, and 4.12 g. 3,17β-dihydroxy-1,3,5-(10)-estratriene 3-(2-benzoyl-4-nitrophenyl) ether (V), m. 97-105°, [α]26D 40°. V was oxidized in excellent yield to III. Further elution of the column with Et2O gave some unreacted IV. V with Ac2O and pyridine gave the acetate (VI) of V, viscous oil. VI (7.5 g.) in 4 cc. glacial AcOH treated slowly with cooling and shaking with 10 cc. cold concentrated H2SO4, kept 0.5 hr. at room temperature, diluted with 40 cc. glacial AcOH, treated dropwise with 10 cc. 1:1 AcOH-30% H2O2, kept 0.5 hr. at room temperature, poured into iced H2O, and filtered gave 4.6 g. 2-OH derivative (VII) of VI, m. 170-2° (MeOH), [α]28.8D 21.0°; 2nd crop, 1.6 g. VII (2.2 g.) in 50 cc. EtOH kept 24 hrs. at 5° with excess CH2N2 in Et2O and evaporated gave 2 g. 2-MeO analog (VIII) of VII, m. 169-71°, [α]26D 36°. VIII (432 mg.) refluxed 1 hr. in 20 cc. pyridine, diluted with 100 cc. C6H6, washed with dilute H2SO4 and N NaOH, evaporated, and the oily residue (446 mg.) chromatographed on 16 g. Al2O3 yielded 180 mg. 2-methoxy-3-hydroxy-17β-acetoxy-1,3,5(10)-estratriene (IX), plates changing to needles, m. 194-6° (C6H6-petr. ether), [α]26D 125°. IX hydrolyzed under N with 5% alc. KOH gave 2-methoxy-17β-estradiol (X), m. 184-6° (C6H6). VIII (1.43 g.) in 50 cc. 6% alc. KOH refluxed 2 hrs. under N, diluted with H2O, and extracted with C6H6 gave 700 mg. X, blades, m. 188-90° (Me2CO), [α]21D 100°; diacetate of X, needles, m. 165-6° (MeOH), [α]26.5D 53°. X partially dissolved in N NaOH and shaken with excess BzCl gave 3-monobenzoate (XI) of X, m. 195-8° (MeOH), [α]28D 72°. VIII (203 mg.) in 40 cc. EtOH containing 8 cc. concentrated H2SO4 refluxed 24 hrs., diluted with H2O, extracted with Et2O, and the extract worked up gave 180 mg. 2-MeO derivative (XII) of V, m. 125-6° (MeOH), [α]28D 61°, also obtained in considerably lower yield by alkaline hydrolysis of VIII at room temperature XII (290 mg.) in 40 cc. Me2CO treated dropwise with 8N CrO3-H2SO4 until an orange-brown color persisted, kept 15 min. at room temperature, poured into H2O, and extracted with CHCl3 yielded 231 mg. 2-MeO derivative (XIII) of I, needles, m. 204-5° (MeOH), [α]28D 89°. XIII (240 mg.) in 20 cc. piperidine refluxed 1 hr., cooled, diluted with 100 cc. C6H6, washed with dilute H2SO4, dried, evaporated, the residual oil subjected to a 99-transfer countercurrent distribution between 70% aqueous MeOH and CCl4, and the combined tubes 14-32 filtered through Al2O3 and crystallized from aqueous MeOH gave 108 mg. 2-methoxyestrone, blades, m. 188-91°, giving with NaOH and BzCl the 3-monobenzoate, needles, m. 225-8°, which was also obtained by oxidation of XI with CrO3.

IT Estra-1,3,5(10)-trien-17β-ol, 3-(2-benzoyl-4-nitrophenoxy)-
Estra-1,3,5(10)-trien-17β-ol, 3-(2-benzoyl-4-nitrophenoxy)-, acetate
Estra-1,3,5(10)-trien-17β-ol, 3-(2-benzoyl-4-nitrophenoxy)-2-methoxy-
Estra-1,3,5(10)-trien-17β-ol, 3-(2-benzoyl-4-nitrophenoxy)-2-methoxy-, acetate

IT 362-07-2, Estradiol, 2-methoxy-

(and derivs.)
IT 362-08-3, Estrone, 2-methoxy- 38781-50-9, Benzophenone, 2-(2,17β-dihydroxyestra-1,3,5(10)-trien-3-yloxy)-5-nitro-, 17-acetate 65932-49-2, Benzophenone, 2-(17β-hydroxyestra-1,3,5(10)-trien-3-yloxy)-5-nitro- 65932-50-5, Benzophenone, 2-(17β-hydroxyestra-1,3,5(10)-trien-3-yloxy)-5-nitro-, acetate 65932-51-6, Benzophenone, 2-(17β-hydroxy-2-methoxyestra-1,3,5(10)-trien-3-yloxy)-5-nitro-, acetate 65932-52-7, Benzophenone, 2-(17β-hydroxy-2-methoxyestra-1,3,5(10)-trien-3-yloxy)-5-nitro- 65932-53-8, Estra-1,3,5(10)-trien-17-one, 3-(2-benzoyl-4-nitrophenoxy)-2-methoxy- 103278-44-0, Estra-1,3,5(10)-trien-17-one, 3-(2-benzoyl-4-nitrophenoxy)- 120024-00-2, Estrone, 2-methoxy-, benzoate
(preparation of)

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L89 ANSWER 1 OF 22 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 2001:916405 HCAPLUS
DN 136:37829
ED Entered STN: 20 Dec 2001
TI Steroids as neurochemical stimulators of the VNO to alleviate pain
IN Berliner, David L.; Monti-Bloch, Luis
PA Pherin Pharmaceuticals, Inc., USA
SO U.S., 286 pp., Cont.-in-part of U.S. Ser. No. 725,862, abandoned.
CODEN: USXXAM
DT Patent
LA English
IC ICM A61K031-56
NCL 514177000
CC 32-6 (Steroids)
Section cross-reference(s): 1, 2, 63
FAN.CNT 12

	PATENT NO.	KIND	DATE		APPLICATION NO.	DATE
PI	US 6331534	B1	20011218		US 1997-919621	19970828 <--
	US 5563131	A	19961008		US 1994-286073	19940804 <--
	US 6066627	A	20000523		US 1996-625268	19960329 <--
	US 6057439	A	20000502		US 1996-686092	19960723 <--
PRAI	US 1994-286073	A2	19940804	<--		
	US 1996-625268	A2	19960329	<--		
	US 1996-686092	A2	19960723	<--		
	US 1996-725862	B2	19961004	<--		

OS MARPAT 136:37829
AB Steroids such as formula I [R1 = oxo, (substituted)OH; R2 = (substituted)alkyl; R3 = H, oxo, halo, (substituted)OH; R4-R12 = independently H, halo, (halo-substituted)methyl; R2R3 may = cyclic ether; R13 = H, Me, methylene, etc.] are prepared Thus, 3α- and 3β-pregna-4,20-dien-3-ols were prepared in 14 and 23% yields, resp., by reduction of pregna-4,20-dien-3-one using lithium trisiamylborohydride in dry THF. The invention relates to a method of alleviating pain. The method comprises nasally administering a steroid which is a human vomeropherin, such that the vomeropherin binds to a specific neuroepithelial receptor. The steroid or steroids is/are preferably administered in the form of a pharmaceutical composition containing one or more pharmaceutically acceptable carriers. Autonomic responses to stimulation of the vomeronasal organ (VNO) by the prepared compds. was measured.
ST steroid prepn neurochem stimulator vomeronasal organ pain
IT Drug delivery systems
(nasal; steroids as neurochem. stimulators of the VNO to alleviate pain)
IT Neurohormone receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)

(neuroepithelial; steroids as neurochem. stimulators of the VNO to alleviate pain)

IT Pain
(steroids as neurochem. stimulators of the VNO to alleviate pain)

IT Steroids, preparation
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(steroids as neurochem. stimulators of the VNO to alleviate pain)

IT Nose
(vomeronasal organ; steroids as neurochem. stimulators of the VNO to alleviate pain)

IT 846-45-7P 1150-90-9P, Estra-1,3,5(10),16-tetraen-3-ol 1224-94-8P 2118-31-2P 4075-07-4P, Androsta-4,16-dien-3-one 28336-31-4P 30505-67-0P **34111-53-0P** 35456-72-5P 65754-63-4P, Pregna-1,4,20-trien-3-one 71496-98-5P, Estra-4,16-dien-3-one 77257-06-8P 86306-95-8P 99898-93-8P 161061-70-7P 161061-73-0P 161061-86-5P 161061-93-4P 161061-95-6P 161061-97-8P 161061-98-9P, Estra-5(10),16-dien-3-one 161062-00-6P 177349-45-0P 177349-47-2P 177349-58-5P, 24-Norchola-4,22-dien-3-one 177349-64-3P 177349-66-5P 177349-74-5P 177794-25-1P 177794-29-5P 177794-30-8P 177856-06-3P 177856-07-4P, Estra-1,3,5(10),6,16-pentaen-3-ol 177856-09-6P 177856-10-9P, Estra-1,3,5(10),7,16-pentaen-3-ol 177856-12-1P 177856-13-2P, Estra-1,3,5,7,9,16-hexaen-3-ol 177856-15-4P 177856-17-6P 177856-20-1P 178688-50-1P 186183-19-7P, 19-Norpregna-5(10),20-dien-3-one 186183-23-3P 186183-25-5P 200511-32-6P 200511-37-1P 200511-39-3P 205994-17-8P 205994-18-9P 205994-19-0P 379738-50-8P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(steroids as neurochem. stimulators of the VNO to alleviate pain)

IT 53-63-4P, Estra-1,3,5(10)-trien-3-ol 472-56-0P 1232-18-4P, Pregn-4-en-3-one 2862-58-0P 2872-90-4P, Androst-4-en-3-one 23062-06-8P 26400-72-6P 35581-65-8P, Pregna-4,16-dien-3-one 58594-49-3P 63014-91-5P, Androsta-4,6,16-trien-3-one 86306-63-0P 86306-96-9P 99898-92-7P, 19-Norpregna-1,3,5(10)-trien-20-yn-3-ol 114611-55-1P, Androsta-4,16-diene-3,6-dione 161061-71-8P 161061-72-9P 161061-77-4P 161061-81-0P 161061-82-1P 161061-83-2P 161061-84-3P 161061-99-0P, Estra-4,9,16-trien-3-one 161062-01-7P 161062-02-8P 161062-04-0P, Estra-1,3,5(10),7-tetraen-3-ol 161062-05-1P 161062-06-2P, Estra-1,3,5(10),6-tetraen-3-ol 161062-08-4P 161062-09-5P 177349-46-1P 177349-48-3P, 24-Norchola-4,20(22)-diene-3,6-dione 177349-49-4P, 24-Norchola-4,20(22)-dien-3-one 177349-54-1P 177349-55-2P 177349-56-3P, Pregna-4,16-diene-3,6-dione 177349-57-4P, Pregna-4,17(20),20-triene-3,6-dione 177349-59-6P 177349-60-9P, 24-Norchola-4,22-diene-3,6-dione 177349-61-0P 177349-63-2P 177349-65-4P 177349-67-6P 177349-68-7P 177349-69-8P 177349-72-3P, Pregna-1,4,20-trien-3-ol 177349-73-4P, Pregna-4,20-diene-3,6-dione 177695-29-3P 177794-21-7P 177794-22-8P 177794-23-9P 177794-24-0P 177794-26-2P 177794-27-3P 177794-31-9P 177794-32-0P 177856-05-2P 177856-08-5P 177856-11-0P 177856-14-3P 177856-16-5P 177856-21-2P 177856-22-3P 177856-23-4P 178033-52-8P, Estra-1,3,5(10),16-tetraene-3,6-diol 186183-17-5P 186183-18-6P 186183-20-0P, 19-Norpregna-5(10),20-dien-3-ol 186183-21-1P 186183-22-2P, 19-Norpregna-4,9,20-trien-3-one 186183-24-4P 186183-26-6P 197094-33-0P 197094-34-1P 200574-68-1P, 19,21-Dinorchol-4-en-3-one 202718-04-5P 205994-20-3P 205994-21-4P 205994-22-5P 205994-23-6P 250683-26-2P, 24-Norchola-5,20(22)-dien-3-one 379738-48-4P 379738-49-5P, Estra-4,6,16-trien-3-ol 379738-51-9P 379738-52-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(steroids as neurochem. stimulators of the VNO to alleviate pain)

IT 53-16-7, reactions 53-43-0 57-63-6 58-22-0 145-13-1 434-22-0
474-86-2 517-09-9 1162-53-4 1576-35-8, p-Toluenesulfonylhydrazide
2208-12-0 2857-45-6 3604-60-2 6228-47-3, Propyltriphenylphosphonium
bromide 13244-39-8 13258-68-9 14030-45-6 14508-15-7,
Pregna-4,20-dien-3-one 17879-91-3 21321-88-0 21321-89-1,
Pregn-4-en-20-yn-3-one 38388-13-5 38978-06-2 39006-59-2 57597-07-6
59452-16-3, 19,21-Dinorchola-1,3,5(10)-trien-3-ol 60149-52-2
60149-53-3, 19-Norpregna-4,20-dien-3-one 63015-08-7,
Androsta-1,4,16-trien-3-one 71716-18-2 93998-04-0 120574-28-9
177349-70-1 177349-71-2 177565-58-1 177794-28-4 178603-56-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(steroids as neurochem. stimulators of the VNO to alleviate pain)

IT 1434-85-1P 19865-18-0P 34988-34-6P 55105-93-6P 103614-70-6P,
Androsta-5,16-dien-3-one 202718-05-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(steroids as neurochem. stimulators of the VNO to alleviate pain)

RE.CNT 125 THERE ARE 125 CITED REFERENCES AVAILABLE FOR THIS RECORD

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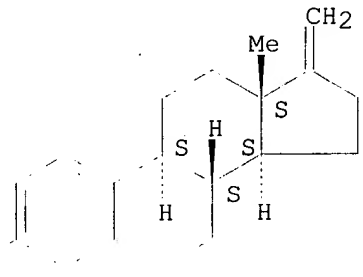
IT **34111-53-0P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(steroids as neurochem. stimulators of the VNO to alleviate pain)

RN 34111-53-0 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-methylene- (7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



L89 ANSWER 2 OF 22 HCAPLUS COPYRIGHT 2003 ACS on STN

AN 2001:283974 HCAPLUS

DN 134:295993

ED Entered STN: 20 Apr 2001

TI Estradiol conjugates and their therapeutic applications

IN Stewart, Alastair George; McAllister, David James; Collis, Maree Patricia; Robertson, Alan Duncan

PA University of Melbourne, Australia

SO PCT Int. Appl., 57 pp.
CODEN: PIXXD2

DT Patent

LA English

IC ICM C07J001-00
ICS A61K047-36; A61K047-42; A61K047-48; A61P009-00; A61P035-00

CC 32-3 (Steroids)
Section cross-reference(s): 1, 2, 33

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	WO 2001027132	A1	20010419	WO 2000-AU1244	20001013	<--
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
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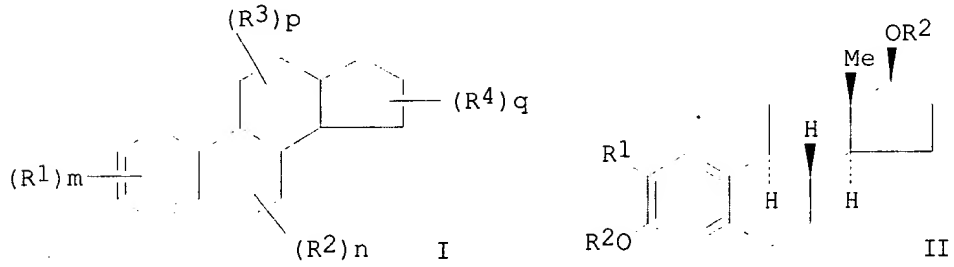
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL					
	JP 2003511461	T2	20030325	JP 2001-530350	20001013	<--
	ZA 2002002622	A	20030304	ZA 2002-2622	20020404	<--
PRAI	AU 1999-3425	A	19991014	<--		
	WO 2000-AU1244	W	20001013	<--		

OS MARPAT 134:295993

GI



AB The invention discloses the preparation of conjugated prodrug of estradiol compound I (R1-R4 = H, OH, halo, alkyl, alkenyl, alkynyl, cycloalkyl, amino, aryl, keto, hydrazono, oximino, carbohydrate, peptide, etc.; m,n,p,q = 0-3), a pharmaceutically acceptable salt or in vivo hydrolyzable ester, amide carbonate or carbamate thereof, in the treatment of conditions associated with enhanced angiogenesis or accelerated cell division, such as cancer, and inflammatory conditions such as asthma and rheumatoid arthritis and hyperproliferative skin disorders including psoriasis. Thus, II [R1 = OMe, R2 = H (III)] was prepared via multi-step reaction sequence starting from β-estradiol II (R1-R2 = H). In human airway fibroblasts thrombin-stimulated increases in cell number were reduced to 12 ± 8% of the control response by III.

ST estradiol conjugate prodrug prepn angiogenesis inhibitor

IT Peptides, preparation
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(conjugates; preparation of peptide conjugated prodrug of estradiol compds. for the treatment of conditions associated with enhanced angiogenesis or accelerated cell division)

IT Partition
(for the measurement of relative solubilities of estradiol conjugates)

IT Glycosides
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(glucuronides, estrogenic; preparation of glucuronide prodrug of estradiol compds. for the treatment of conditions associated with enhanced angiogenesis or accelerated cell division)

IT Estrogens
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(hydroxy, glucuronides; preparation of glucuronide prodrug of estradiol compds. for the treatment of conditions associated with enhanced angiogenesis or accelerated cell division)

IT Fluorometry
(in determination of relative solubilities of estradiol conjugates for the treatment of conditions associated with enhanced angiogenesis or accelerated cell division)

IT Antitumor agents
(preparation of conjugated prodrug of estradiol compds. for the treatment of conditions associated with enhanced angiogenesis or accelerated cell division)

IT Antiasthmatics
Rheumatoid arthritis
(preparation of conjugated prodrug of estradiol compds. for the treatment of inflammatory conditions such as asthma and rheumatoid arthritis)

IT Psoriasis
(preparation of conjugated prodrug of estradiol compds. for the treatment psoriasis)

IT Estrogen receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(preparation of estradiol conjugates and their binding with rat uterine cytosol estrogen receptor)

IT DNA formation
(preparation of estradiol conjugates for regulation of DNA synthesis)

IT Respiratory tract
(preparation of estradiol conjugates for regulation of airway mesenchymal cell number)

IT Angiogenesis inhibitors
Anti-inflammatory agents
(preparation of estradiol conjugates for the treatment of conditions associated with enhanced angiogenesis or accelerated cell division)

IT Estrogens
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of estradiol conjugates for the treatment of conditions associated with enhanced angiogenesis or accelerated cell division)

IT Galactosides
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of galactoside prodrug of estradiol compds. for the treatment of conditions associated with enhanced angiogenesis or accelerated cell division)

IT Drug delivery systems
(prodrugs; preparation of conjugated prodrug of an estradiol compds. for the treatment of conditions associated with enhanced angiogenesis or

accelerated cell division)
IT Proliferation inhibition
(proliferation inhibitors; preparation of estradiol conjugates for the treatment of conditions associated with enhanced angiogenesis or accelerated cell division)
IT Skin, disease
(proliferative; preparation of conjugated prodrug of estradiol compds. for the treatment of hyperproliferative skin disorders)
IT **7291-57-8P** 69540-62-1P 334791-42-3P 334791-45-6P 334791-46-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of estradiol conjugates for the treatment of conditions associated
with enhanced angiogenesis or accelerated cell division)
IT 171064-21-4P 334791-43-4P 334791-47-8P 334791-49-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of estradiol conjugates for the treatment of conditions associated
with enhanced angiogenesis or accelerated cell division)
IT 9001-45-0, β-Glucuronidase
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(preparation of estradiol conjugates for the treatment of conditions associated
with enhanced angiogenesis or accelerated cell division)
IT 52717-98-3P
RL: BYP (Byproduct); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of estradiol conjugates for the treatment of conditions associated
with enhanced angiogenesis or accelerated cell division)
IT 513-78-0, Cadmium carbonate
RL: CAT (Catalyst use); USES (Uses)
(preparation of estradiol conjugates for the treatment of conditions associated
with enhanced angiogenesis or accelerated cell division)
IT 50-28-2, β-Estradiol, reactions 100-39-0, Benzyl bromide 108-24-7, Acetic anhydride 3068-32-4 7803-57-8, Hydrazine hydrate 21085-72-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of estradiol conjugates for the treatment of conditions associated
with enhanced angiogenesis or accelerated cell division)
IT 362-07-2P 69455-04-5P 69540-63-2P 83274-89-9P 159143-75-6P 159143-76-7P 192062-05-8P 334791-44-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of estradiol conjugates for the treatment of conditions associated
with enhanced angiogenesis or accelerated cell division)
RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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(2) Holler, M; Acta Endocrinologica 1982, V100, P57 MEDLINE
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(5) Nambara, T; Chem Pharm Bull 1977, V25(5), P942 HCAPLUS
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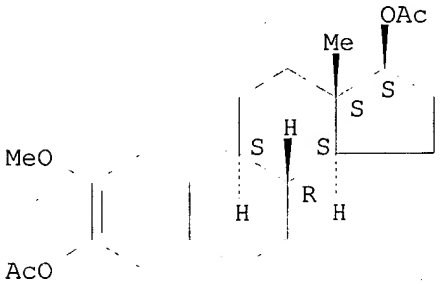
(9) Stalford, A; Steroids 1997, V62, P750 HCAPLUS
(10) Takanashi, K; Bunseki Kagaku 1995, V44(10), P793 HCAPLUS
(11) The Children'S Medical Center Corporation; WO 9504535 1995 HCAPLUS
(12) Watanabe, K; Chem Pharm Bull 1982, V30(9), P3231 HCAPLUS

IT **7291-57-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of estradiol conjugates for the treatment of conditions associated
with enhanced angiogenesis or accelerated cell division)
RN 7291-57-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-, diacetate, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L89 ANSWER 3 OF 22 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 2000:635218 HCAPLUS
DN 133:208036
ED Entered STN: 13 Sep 2000
TI Preparation of steroids as neurochemical stimulators of the VNO to alleviate symptoms of PMS and anxiety
IN Jennings-white, Clive L.; Berliner, David L.; Adams, Nathan W.; Monti-bloch, Luis
PA Pherin Pharmaceuticals, Inc., USA
SO U.S., 299 pp., Cont.-in-part of U.S. Ser. No. 725,862.
CODEN: USXXAM
DT Patent
LA English
IC ICM A61K031-56
NCL 514177000
CC 32-3 (Steroids)
Section cross-reference(s): 2, 63
FAN.CNT 12

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	US 6117860	A	20000912	US 1997-899094	19970723	<--
	US 5563131	A	19961008	US 1994-286073	19940804	<--
	US 6066627	A	20000523	US 1996-625268	19960329	<--
	US 6057439	A	20000502	US 1996-686092	19960723	<--
	WO 9814194	A1	19980409	WO 1997-US18086	19971006	<--

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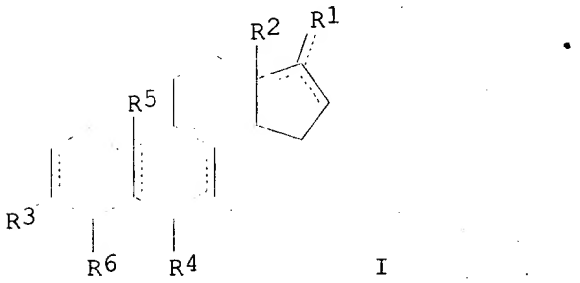
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

AU 9748103 A1 19980424 AU 1997-48103 19971006 <--

PRAI US 1994-286073 A2 19940804 <--
US 1996-625268 A2 19960329 <--
US 1996-686092 A2 19960723 <--
US 1996-725862 A2 19961004 <--
US 1997-899094 A 19970723 <--
WO 1997-US18086 W 19971006 <--

OS MARPAT 133:208036

GI



I

AB The invention relates to a method of alleviating the symptoms of PMS and anxiety. The method comprises nasally administering a steroid which is a human vomeropherin, e.g. a compound of formula I [R1 = H, Me, CH2, halo; R2 = absent, H, Me; R3 = oxo, OH, alkoxy, acyloxy, benzoyl, etc.; R4 = H, OH, alkoxy, acyloxy, oxo, halo; R5 = absent, H, OH, alkoxy, acyloxy; R6 = H, halo], such that the vomeropherin binds to a specific neuroepithelial receptor. Thus, 10β-hydroxy-16α,17α-epoxyestr-4-en-3-one is prepared from estra 5(10),16-dien-3-one, and is used in pharmaceutical compns. The compds. of the invention are tested for their effect on EEG and autonomic activity in women and men. The steroid or steroids is/are preferably administered in the form of a pharmaceutical composition containing one or more pharmaceutically acceptable carriers.

ST steroid prepn neurochem stimulator VNO; estrene prepn neurochem stimulator VNO; PMS treatment steroid prepn; premenstrual dysphoric disorder treatment steroid prepn; anxiety treatment steroid prepn; neuroepithelial receptor steroid prepn

IT Reflex
(autonomic; preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)

IT Brain
(hypothalamus; preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)

IT Fertility
(inhibitors; preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)

IT Drug delivery systems
(nasal; preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)

IT Receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(neuroepithelial; preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)

IT Ovarian cycle
(premenstrual syndrome, treatment; preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)
IT Antitumor agents
Anxiolytics
(preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)
IT Steroids, preparation
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)
IT Nose
(vomeronasal organ; preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)
IT 1150-90-9P, Estra-1,3,5(10),16-tetraen-3-ol 4736-62-3P 35581-65-8P, Pregna-4,16-dien-3-one 65754-63-4P, Pregna-1,4,20-trien-3-one 71496-98-5P, Estra-4,16-dien-3-one 97560-70-8P, 19-Norpregna-1,3,5(10),20-tetraen-3-ol 99898-92-7P, 19-Norpregna-1,3,5(10)-trien-20-yn-3-ol 99898-93-8P 105663-60-3P 161061-73-0P 161061-81-0P 161061-82-1P 177349-45-0P 177349-52-9P 177349-64-3P 177349-66-5P 177565-58-1P 186183-19-7P, 19-Norpregna-5(10),20-dien-3-one 186183-25-5P 250683-25-1P
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(preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)
IT 2118-31-2 14030-45-6 14508-15-7, Pregna-4,20-dien-3-one 16377-13-2 21321-88-0 28336-31-4 60149-52-2 60149-53-3, 19-Norpregna-4,20-dien-3-one 71016-68-7 93998-04-0 177349-71-2 202718-08-9 202718-10-3 205994-34-9
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)
IT 472-56-0P 1232-18-4P, Pregn-4-en-3-one 2862-58-0P, Pregn-5-en-3β-ol 21321-95-9P 23062-06-8P 23640-47-3P 26400-72-6P 30505-67-0P 58594-49-3P 71716-18-2P 86306-63-0P 86306-96-9P 120476-05-3P 161061-71-8P 161061-72-9P 161061-83-2P 161061-84-3P 161061-99-0P, Estra-4,9,16-trien-3-one 161062-01-7P 161062-02-8P 161062-04-0P, Estra-1,3,5(10),7-tetraen-3-ol 161062-05-1P 161062-09-5P 177349-46-1P 177349-48-3P, 24-Norchola-4,20(22)-diene-3,6-dione 177349-49-4P, 24-Norchola-4,20(22)-dien-3-one 177349-53-0P 177349-54-1P 177349-55-2P 177349-56-3P, Pregna-4,16-diene-3,6-dione 177349-57-4P, Pregna-4,17(20),20-triene-3,6-dione 177349-59-6P 177349-60-9P, 24-Norchola-4,22-diene-3,6-dione 177349-61-0P 177349-62-1P 177349-63-2P 177349-65-4P 177349-67-6P 177349-68-7P 177349-69-8P 177349-72-3P, Pregna-1,4,20-trien-3-ol 177349-73-4P, Pregna-4,20-diene-3,6-dione 177695-29-3P 177794-21-7P 177794-22-8P 177794-23-9P 177794-24-0P 177794-26-2P 177794-27-3P 177794-31-9P 177794-32-0P 177856-08-5P 177856-11-0P 177856-14-3P 177856-16-5P 177856-19-8P 177856-20-1P 177856-21-2P 177856-22-3P 177856-23-4P 178033-52-8P, Estra-1,3,5(10),16-tetraene-3,6-diol 178033-53-9P, Estra-4,16-dien-3-ol 186183-17-5P 186183-18-6P 186183-21-1P 186183-22-2P, 19-Norpregna-4,9,20-trien-3-one 186183-26-6P 186183-27-7P 186183-28-8P 186183-29-9P 190596-13-5P, Estra-5(10),16-dien-3-ol 200511-34-8P 200574-68-1P, 19,21-Dinorchol-4-en-3-one 202718-04-5P 211123-94-3P 265313-78-8P 265313-81-3P 265313-82-4P 265313-83-5P 265313-84-6P 265313-85-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)

IT 53-16-7, Estrone, reactions 53-43-0 57-63-6, Ethynylestradiol 58-22-0, Testosterone 145-13-1 434-22-0, 19-Nortestosterone 474-86-2, Equilin 517-09-9, Equilenin 1162-53-4 1624-62-0 2208-12-0, 6-Dehydroestrone 2857-45-6 3604-60-2 13244-39-8 13258-68-9, Ethynylestradiol diacetate 16397-00-5 17879-91-3 21321-89-1, Pregn-4-en-20-yn-3-one 33767-87-2 38388-13-5 38978-06-2 39006-59-2 57597-07-6 63015-08-7, Androsta-1,4,16-trien-3-one 120574-28-9 177349-70-1 178603-56-0 215732-74-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)

IT 846-45-7P 1224-94-8P 4075-07-4P, Androsta-4,16-dien-3-one 7628-02-6P 19865-18-0P **34111-53-0P** 34988-34-6P 35456-72-5P 55105-93-6P, Estrone p-toluenesulfonylhydrazone 59452-16-3P, 19,21-Dinorchola-1,3,5(10)-trien-3-ol 71683-67-5P 77257-06-8P 86306-95-8P 103614-70-6P, Androsta-5,16-dien-3-one 105644-55-1P 161061-70-7P 161061-86-5P 161061-93-4P 161061-95-6P 161061-97-8P 161061-98-9P, Estra-5(10),16-dien-3-one 161062-00-6P 177349-50-7P 177349-51-8P 177349-58-5P, 24-Norchola-4,22-dien-3-one 177349-74-5P 177794-25-1P 177794-29-5P 177794-30-8P 177856-06-3P 177856-07-4P, Estra-1,3,5(10),6,16-pentaen-3-ol 177856-09-6P 177856-10-9P, Estra-1,3,5(10),7,16-pentaen-3-ol 177856-12-1P 177856-13-2P, Estra-1,3,5,7,9,16-hexaen-3-ol 177856-15-4P 177856-17-6P 177856-18-7P 178688-50-1P 178688-52-3P 200511-32-6P 200511-37-1P 200511-39-3P 200511-50-8P, 19,21-Dinorchola-5(10),16-dien-3-one 202718-11-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)

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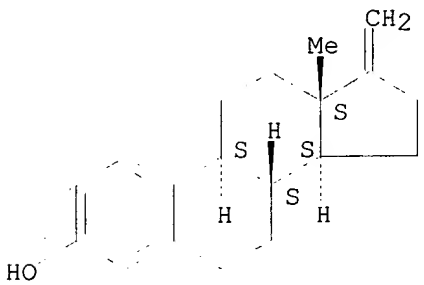
IT **34111-53-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)
RN 34111-53-0 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methylene- (7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



L89 ANSWER 4 OF 22 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 2000:344112 HCAPLUS
DN 132:347795
ED Entered STN: 24 May 2000
TI Preparation of steroids as neurochemical initiators of change in human blood levels of LH
IN Jennings-White, Clive L.; Berliner, David L.; Adams, Nathan W.
PA Pherin Corporation, USA
SO U.S., 255 pp., Cont.-in-part of U.S. 5,563,131.
CODEN: USXXAM
DT Patent
LA English
IC ICM A61K031-56
NCL 514177000
CC 32-5 (Steroids)
Section cross-reference(s): 2
FAN.CNT 12

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	WO 9736596	A1	19971009	WO 1997-US6061	19970328	<--

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LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT,
RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB,
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ML, MR, NE, SN, TD, TG

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OS MARPAT 132:347795

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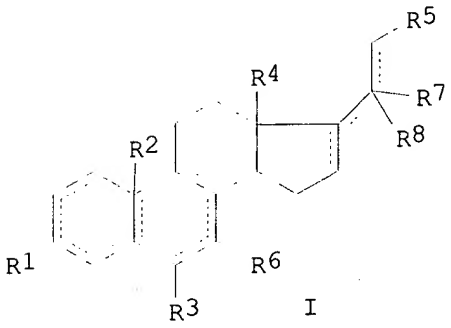

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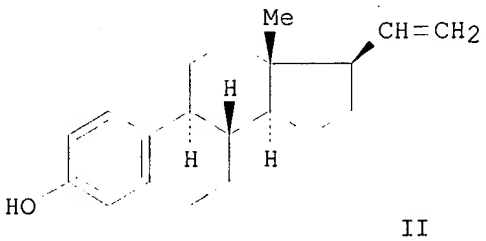

II

AB The invention relates to a method of altering the blood levels of LH or FSH in an individual. The method comprises nasally administering a steroid which is a human vomeropherin, such that the vomeropherin binds to a specific neuroepithelial receptor. Steroids, e.g. of formula I [R1 = oxo, OH, OAc, propionyloxy, alkoxy, acyloxy, benzyloxy; R2 = H, OH, alkoxy, absent; R3 = oxo, OH, alkoxy, halo; R4 = Me, Et; R5 = H, Me, halo; R6 = H, Me; R7, R8 = H, halo, absent], are prepared as vomeropherins. Thus, II was prepared from ethynylestradiol diacetate. The prepared 19-norpregnane vomeropherins were tested for autonomic activity in women.

ST neurochem initiator LH blood level steroid prepn; FSH blood level neurochem initiator steroid prepn; anxiolytic steroid vomeropherin prepn; hypothalamic function steroid vomeropherin prepn

IT Brain
(hypothalamus; preparation of steroids as neurochem. initiators of change in human blood levels of LH)

IT Fertility
(inhibitors; preparation of steroids as neurochem. initiators of change in human blood levels of LH)

IT Drug delivery systems
(nasal; preparation of steroids as neurochem. initiators of change in human blood levels of LH)

IT Anxiolytics
(preparation of steroids as neurochem. initiators of change in human blood levels of LH)

IT Steroids, preparation
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of steroids as neurochem. initiators of change in human blood levels of LH)

IT Nose
(vomeronasal organ; preparation of steroids as neurochem. initiators of change in human blood levels of LH)

IT 846-45-7P 1150-90-9P, Estra-1,3,5(10),16-tetraen-3-ol 1224-94-8P 4075-07-4P, Androsta-4,16-dien-3-one **34111-53-0P** 35456-72-5P 65754-63-4P, Pregna-1,4,20-trien-3-one 71496-98-5P, Estra-4,16-dien-3-one 77257-06-8P 86306-95-8P 97560-70-8P, 19-Norpregna-1,3,5(10),20-tetraen-3-ol 99898-93-8P 161061-70-7P 161061-73-0P 161061-86-5P 161061-93-4P 161061-95-6P 161061-97-8P 161061-98-9P, Estra-5(10),16-dien-3-one 161062-00-6P 177349-45-0P 177349-50-7P 177349-51-8P 177349-52-9P 177349-58-5P, 24-Norchola-4,22-dien-3-one 177349-64-3P 177349-66-5P 177349-74-5P 177565-58-1P 177794-25-1P 177794-29-5P 177794-30-8P 177856-06-3P 177856-07-4P, Estra-1,3,5(10),6,16-pentaen-3-ol 177856-09-6P 177856-10-9P, Estra-1,3,5(10),7,16-pentaen-3-ol 177856-12-1P 177856-13-2P, Estra-1,3,5,7,9,16-hexaen-3-ol 177856-15-4P 177856-17-6P 177856-18-7P 186183-19-7P, 19-Norpregna-5(10),20-dien-3-one 186183-25-5P 250683-25-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of steroids as neurochem. initiators of change in human blood levels of LH)

IT 2118-31-2 14030-45-6 14508-15-7, Pregna-4,20-dien-3-one 21321-88-0 28336-31-4 60149-52-2 60149-53-3, 19-Norpregna-4,20-dien-3-one 71716-18-2
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(preparation of steroids as neurochem. initiators of change in human blood levels of LH)

IT 53-63-4P, Estra-1,3,5(10)-trien-3-ol 1232-18-4P, Pregn-4-en-3-one 2862-58-0P, Pregn-5-en-3β-ol 2872-90-4P, Androst-4-en-3-one 4736-62-3P 21321-95-9P 23062-06-8P 26400-72-6P 30505-67-0P 58594-49-3P 59077-04-2P, 19-Norpregna-1,3,5(10)-trien-3-ol 63014-91-5P, Androsta-4,6,16-trien-3-one 86306-63-0P 86306-96-9P 99898-92-7P, 19-Norpregna-1,3,5(10)-trien-20-yn-3-ol 114611-55-1P, Androsta-4,16-diene-3,6-dione 161061-71-8P 161061-72-9P 161061-81-0P 161061-82-1P 161061-83-2P 161061-84-3P 161061-99-0P, Estra-4,9,16-trien-3-one 161062-01-7P 161062-02-8P 161062-04-0P, Estra-1,3,5(10),7-tetraen-3-ol 161062-05-1P 161062-06-2P, Estra-1,3,5(10),6-tetraen-3-ol 161062-08-4P 161062-09-5P 177349-46-1P 177349-48-3P, 24-Norchola-4,20(22)-diene-3,6-dione 177349-49-4P, 24-Norchola-4,20(22)-dien-3-one 177349-53-0P 177349-54-1P 177349-55-2P 177349-56-3P, Pregna-4,16-diene-3,6-dione 177349-57-4P, Pregna-4,17(20),20-triene-3,6-dione 177349-59-6P 177349-60-9P, 24-Norchola-4,22-diene-3,6-dione 177349-61-0P 177349-62-1P 177349-63-2P 177349-65-4P 177349-67-6P 177349-68-7P 177349-69-8P 177349-72-3P, Pregna-1,4,20-trien-3-ol 177349-73-4P, Pregna-4,20-diene-3,6-dione 177695-29-3P 177794-21-7P 177794-22-8P 177794-23-9P 177794-24-0P 177794-26-2P 177794-27-3P 177794-31-9P 177794-32-0P 177856-05-2P 177856-08-5P 177856-11-0P 177856-14-3P 177856-16-5P 177856-19-8P 177856-20-1P 177856-21-2P 177856-22-3P 177856-23-4P 186183-17-5P 186183-18-6P 186183-21-1P 186183-22-2P, 19-Norpregna-4,9,20-trien-3-one 186183-26-6P 186183-27-7P 186183-28-8P 186183-29-9P 197094-33-0P 197094-34-1P 211123-94-3P

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(preparation of steroids as neurochem. initiators of change in human blood levels of LH)

IT 9002-67-9, LH 9002-68-0, FSH
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(preparation of steroids as neurochem. initiators of change in human blood levels of LH)

IT 53-16-7, Estrone, reactions 53-43-0 57-63-6, Ethynylestradiol
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474-86-2, Equilin 517-09-9, Equilenin 1162-53-4 2208-12-0,
6-Dehydroestrone 2857-45-6 3604-60-2, Ethynylandrostenediol
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57597-07-6 63015-08-7, Androsta-1,4,16-trien-3-one 93998-04-0
177349-70-1 177349-71-2 177794-28-4 178603-56-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of steroids as neurochem. initiators of change in human blood levels of LH)

IT 19865-18-0P 33767-87-2P 34988-34-6P 55105-93-6P, Estrone p-toluenesulfonylhydrazone 103614-70-6P, Androsta-5,16-dien-3-one
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of steroids as neurochem. initiators of change in human blood levels of LH)

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(32) Bull, J; J Chem Soc Perkin I 1977, V7, P724
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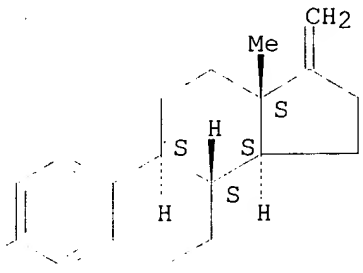
(40) Prezewowsky; US 3682983 1972 HCAPLUS

IT **34111-53-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of steroids as neurochem. initiators of change in human blood levels of LH)
RN 34111-53-0 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methylene- (7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



L89 ANSWER 5 OF 22 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 2000:284021 HCAPLUS
DN 132:308544
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TI Preparation of steroids as neurochemical stimulators of the VNO to alleviate symptoms of PMS and anxiety
IN Jennings-white, Clive L.; Berliner, David L.; Adams, Nathan W.; Monti-bloch, Luis
PA Pherin Corporation, USA
SO U.S., 284 pp., Cont.-in-part of U.S. Ser. No. 625,268.
CODEN: USXXAM
DT Patent
LA English
IC ICM C07J005-00
NCL 540024000
CC 32-3 (Steroids)
Section cross-reference(s): 2, 63
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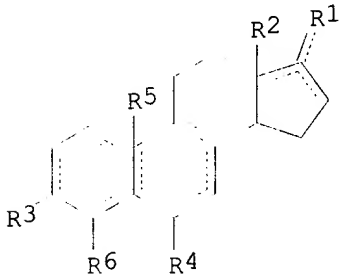

I

AB The invention relates to a method of alleviating the symptoms of PMS and anxiety. The method comprises nasally administering a steroid which is a human vomeropherin, e.g. a compound of formula I [R1 = H, Me, CH2, halo; R2 = absent, H, Me; R3 = oxo, OH, alkoxy, acyloxy, benzoyl, etc.; R4 = H, OH, alkoxy, acyloxy, oxo, halo; R5 = absent, H, OH, alkoxy, acyloxy; R6 = H, halo], such that the vomeropherin binds to a specific neuroepithelial receptor. Thus, 10β-hydroxy-16α,17α-epoxyestr-4-en-3-one is prepared from estra 5(10),16-dien-3-one, and is used in pharmaceutical compns. The compds. of the invention are tested for their effect on EEG and autonomic activity in women and men. The steroid or steroids is/are preferably administered in the form of a pharmaceutical composition containing one or more pharmaceutically acceptable carriers.

ST steroid prepn neurochem stimulator VNO; estrene prepn neurochem stimulator VNO; PMS treatment steroid prepn; premenstrual disphoric disorder treatment steroid prepn; anxiety treatment steroid prepn; neuroepithelial receptor steroid prepn

IT Reflex
(autonomic; preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)

IT Brain
(hypothalamus; preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)

IT Fertility
(inhibitors; preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)
IT Drug delivery systems
(nasal; preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)
IT Receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(neuroepithelial; preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)
IT Ovarian cycle
(premenstrual syndrome, treatment; preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)
IT Antitumor agents
Anxiolytics
(preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)
IT Steroids, preparation
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)
IT Nose
(vomeronasal organ; preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)
IT 1150-90-9P, Estra-1,3,5(10),16-tetraen-3-ol 65754-63-4P, Pregna-1,4,20-trien-3-one 71496-98-5P, Estra-4,16-dien-3-one 97560-70-8P, 19-Norpregna-1,3,5(10),20-tetraen-3-ol 99898-92-7P, 19-Norpregna-1,3,5(10)-trien-20-yn-3-ol 99898-93-8P 161061-73-0P 161061-81-0P 161061-82-1P 177349-45-0P 177349-52-9P 177349-64-3P 177349-66-5P 177565-58-1P 186183-19-7P, 19-Norpregna-5(10),20-dien-3-one 186183-25-5P 250683-25-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)
IT 2118-31-2 14030-45-6 14508-15-7, Pregna-4,20-dien-3-one 21321-88-0 28336-31-4 60149-52-2 60149-53-3, 19-Norpregna-4,20-dien-3-one 93998-04-0 177349-71-2
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)
IT 472-56-0P 1232-18-4P, Pregn-4-en-3-one 2862-58-0P, Pregn-5-en-3β-ol 4736-62-3P 21321-95-9P 23062-06-8P 23640-47-3P 26400-72-6P 30505-67-0P 35581-65-8P, Pregna-4,16-dien-3-one 58594-49-3P 71716-18-2P 86306-63-0P 86306-96-9P 120476-05-3P 161061-71-8P 161061-72-9P 161061-83-2P 161061-84-3P 161061-99-0P, Estra-4,9,16-trien-3-one 161062-01-7P 161062-02-8P 161062-04-0P, Estra-1,3,5(10),7-tetraen-3-ol 161062-05-1P 161062-09-5P 177349-46-1P 177349-48-3P, 24-Norchola-4,20(22)-diene-3,6-dione 177349-49-4P, 24-Norchola-4,20(22)-dien-3-one 177349-53-0P 177349-54-1P 177349-55-2P 177349-56-3P, Pregna-4,16-diene-3,6-dione 177349-57-4P, Pregna-4,17(20),20-triene-3,6-dione 177349-59-6P 177349-60-9P, 24-Norchola-4,22-diene-3,6-dione 177349-61-0P 177349-62-1P 177349-63-2P 177349-65-4P 177349-67-6P 177349-68-7P 177349-69-8P 177349-72-3P, Pregna-1,4,20-trien-3-ol 177349-73-4P, Pregna-4,20-diene-3,6-dione 177695-29-3P 177794-21-7P 177794-22-8P

177794-23-9P 177794-24-0P 177794-26-2P 177794-27-3P 177794-31-9P
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177856-19-8P 177856-20-1P 177856-21-2P 177856-22-3P 177856-23-4P
178033-52-8P, Estra-1,3,5(10),16-tetraene-3,6-diol 178033-53-9P,
Estra-4,16-dien-3-ol 186183-17-5P 186183-18-6P 186183-21-1P
186183-22-2P, 19-Norpregna-4,9,20-trien-3-one 186183-26-6P
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265313-81-3P 265313-82-4P 265313-83-5P 265313-84-6P 265313-85-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)

IT 53-16-7, Estrone, reactions 53-43-0 57-63-6, Ethynylestradiol
58-22-0, Testosterone 145-13-1 434-22-0, 19-Nortestosterone
474-86-2, Equilin 517-09-9, Equilenin 1162-53-4 2208-12-0,
6-Dehydroestrone 2857-45-6 3604-60-2 13244-39-8 13258-68-9,
Ethynylestradiol diacetate 17879-91-3 21321-89-1, Pregn-4-en-20-yn-3-one 33767-87-2 38388-13-5 38978-06-2 39006-59-2 57597-07-6
63015-08-7, Androsta-1,4,16-trien-3-one 120574-28-9 177349-70-1
178603-56-0 215732-74-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)

IT 846-45-7P 1224-94-8P 4075-07-4P, Androsta-4,16-dien-3-one
19865-18-0P **34111-53-0P** 34988-34-6P 35456-72-5P
55105-93-6P, Estrone p-toluenesulfonylhydrazone 59452-16-3P,
19,21-Dinorchola-1,3,5(10)-trien-3-ol 77257-06-8P 86306-95-8P
103614-70-6P, Androsta-5,16-dien-3-one 161061-70-7P 161061-86-5P
161061-93-4P 161061-95-6P 161061-97-8P 161061-98-9P,
Estra-5(10),16-dien-3-one 161062-00-6P 177349-50-7P 177349-51-8P
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177794-29-5P 177794-30-8P 177856-06-3P 177856-07-4P,
Estra-1,3,5(10),6,16-pentaen-3-ol 177856-09-6P 177856-10-9P,
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Estra-1,3,5,7,9,16-hexaen-3-ol 177856-15-4P 177856-17-6P
177856-18-7P 178688-50-1P 200511-32-6P 200511-37-1P 200511-39-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)

RE.CNT 119 THERE ARE 119 CITED REFERENCES AVAILABLE FOR THIS RECORD
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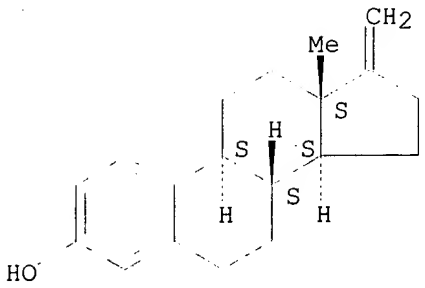
IT **34111-53-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of steroids as neurochem. stimulators of VNO to alleviate symptoms of PMS and anxiety)

RN 34111-53-0 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methylene- (7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



L89 ANSWER 6 OF 22 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 1999:460438 HCAPLUS
DN 131:88083
ED Entered STN: 28 Jul 1999
TI Preparation of estrone sulfamate inhibitors of estrone sulfatase
IN Tanabe, Masato; Peters, Richard H.; Chao, Wan-Ru; Shigeno, Kazuhiko
PA SRI International, USA
SO PCT Int. Appl., 102 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07J041-00
ICS A61K031-565; A61K031-57; A61K031-575
CC 32-3 (Steroids)
Section cross-reference(s): 2, 63
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
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	CA 2318349	AA	19990708	CA 1998-2318349	19981221 <--
	AU 9919416	A1	19990719	AU 1999-19416	19981221 <--
	AU 751732	B2	20020829		
	EP 1042354	A2	20001011	EP 1998-964243	19981221 <--
	R: DE, FR, GB, IT, NL				
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PRAI	US 1997-997416	A	19971224 <--		
	WO 1998-US27333	W	19981221 <--		

OS MARPAT 131:88083
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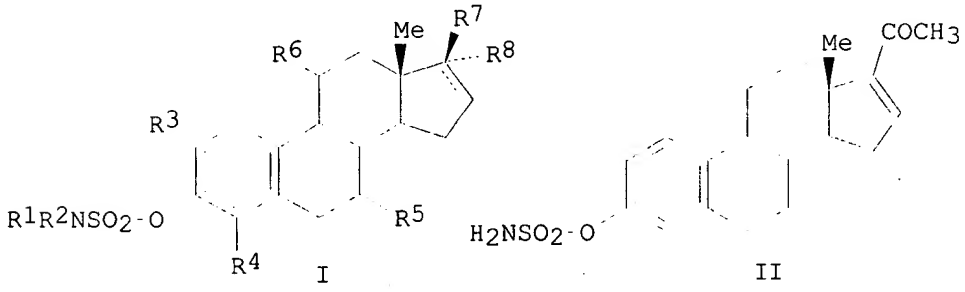

AB Novel compds.of formula I [R1, R2 = H, alkyl, etc.; R3 = H, CN, NO2, COOH,

alkoxycarbonyl, etc.; R4 = H, NO2, (substituted) amino; R5, R6 = H, alkyl; R7, R8 = H, alkyl, alkenyl, alkynyl, alkoxy, acyl, acyloxy, etc.; R7,R8 = oxo, alkylidene, etc.] are prepared as inhibitors of estrone sulfatase. Thus, II is prepared from ethynylestradiol in 4 steps. and showed estrone sulfatase inhibitory activity of IC50 = 21 pM. Pharmaceutical compns. and methods for using I to treat estrogen-dependent disorders are provided.

ST estrone sulfamate prepn estrone sulfatase inhibitor

IT Estrogens
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(antiestrogens; preparation of estrone sulfamates as inhibitors of estrone sulfatase)

IT Antitumor agents
(preparation of estrone sulfamates as inhibitors of estrone sulfatase)

IT 59298-96-3, Estrone sulfatase
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(inhibitors; preparation of estrone sulfamates as inhibitors of estrone sulfatase)

IT 185910-34-3P 185910-42-3P 208924-86-1P 208924-87-2P 229485-78-3P
229485-79-4P 229485-80-7P 229485-81-8P 229485-82-9P 229485-83-0P
229485-84-1P 229485-85-2P 229485-86-3P 229485-87-4P 229485-88-5P
229485-89-6P 229485-90-9P 229485-91-0P 229485-92-1P 229485-93-2P
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229485-99-8P 229486-00-4P 229486-01-5P 229486-02-6P 229486-03-7P
229486-04-8P 229486-05-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of estrone sulfamates as inhibitors of estrone sulfatase)

IT 50-28-2, Estradiol, reactions 53-16-7, Estrone, reactions 57-63-6, Ethynylestradiol 108-01-0, N,N-Dimethylethanolamine 109-77-3, Malononitrile 362-08-3 867-13-0, Triethylphosphonoacetate 1779-51-7, Butyltriphenylphosphonium bromide 4584-46-7 5407-04-5 6228-47-3, Propyltriphenylphosphonium bromide 7678-95-7 67530-18-1 229486-27-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of estrone sulfamates as inhibitors of estrone sulfatase)

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59452-15-2P 59452-16-3P, 19,21-Dinorchola-1,3,5(10)-trien-3-ol
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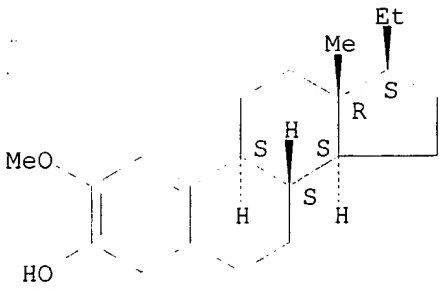
206442-55-9P 208758-44-5P 208758-45-6P 208758-46-7P 208758-49-0P
208758-50-3P 229486-06-0P 229486-07-1P 229486-08-2P 229486-09-3P
229486-10-6P 229486-11-7P 229486-12-8P 229486-13-9P 229486-14-0P
229486-15-1P 229486-16-2P 229486-17-3P **229486-18-4P**
229486-19-5P 229486-20-8P 229486-21-9P 229486-22-0P 229486-23-1P
229486-24-2P 229486-25-3P 229486-26-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of estrone sulfamates as inhibitors of estrone sulfatase)

IT **229486-18-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of estrone sulfamates as inhibitors of estrone sulfatase)

RN 229486-18-4 HCAPLUS

CN 19-Norpregna-1,3,5(10)-trien-3-ol, 2-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

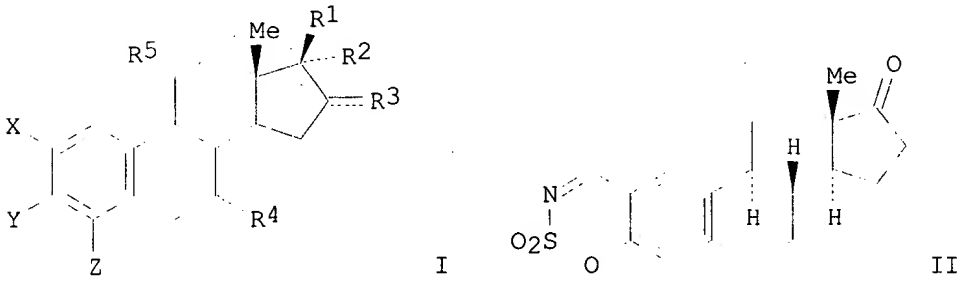


L89 ANSWER 7 OF 22 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 1998:397783 HCAPLUS
DN 129:54482
ED Entered STN: 29 Jun 1998
TI Preparation of steroid inhibitors of estrone sulfatase and associated pharmaceutical compositions and methods of use
IN Tanabe, Masato; Peters, Richard H.; Chao, Wan-ru; Shigeno, Kazuhiko
PA SRI International, USA
SO U.S., 23 pp.
CODEN: USXXAM
DT Patent
LA English
IC ICM A61K031-58
ICS C07J071-00
NCL 514176000
CC 32-3 (Steroids)
Section cross-reference(s): 1, 2
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 5763432	A	19980609	US 1997-794229	19970129 <--
US 5861388	A	19990119	US 1997-1601	19971231 <--
WO 9832763	A1	19980730	WO 1998-US1846	19980129 <--

W: CA, JP, KR
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

PRAI US 1997-794229 19970129 <--
OS MARPAT 129:54482
GI



AB Estratriene derivs. of formula I [X and Y, or Y and Z, form an oxathiazine dioxide ring or a dihydro-oxathiazine dioxide ring; R1, R2 = H, alkyl, alkynyl, (substituted) OH; R1R2 = O, S, (substituted) CH2; R3 = H, halo, alkyl, CH2; R4 = H, alkyl; R5 = H, OH, alkyl, alkenyl, alkoxy, aryl, CH2] are prepared as inhibitors of estrone sulfatase. Pharmaceutical compns. and methods for using I to treat estrogen-dependent disorders are provided as

well. Thus, estradiol is transformed into II in 3 steps. In an estrone sulfatase inhibition assay, II showed 5-% inhibition at 9.3 nM.

ST estratriene deriv prepn estrone sulfatase inhibitor

IT 208758-20-7P 208758-22-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of steroid inhibitors of estrone sulfatase)

IT 208758-16-1P 208758-17-2P 208758-21-8P 208758-23-0P 208758-25-2P
208758-33-2P 208758-34-3P 208758-35-4P 208758-36-5P 208758-37-6P
208758-38-7P 208758-39-8P 208758-41-2P 208758-43-4P 208758-48-9P
208758-52-5P 208758-54-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of steroid inhibitors of estrone sulfatase)

IT 59298-96-3, Estrone sulfatase
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(preparation of steroid inhibitors of estrone sulfatase)

IT 50-28-2, Estradiol, reactions 53-16-7, Estrone, reactions 57-63-6, 17α-Ethynylestradiol 1530-32-1, Ethyltriphenylphosphonium bromide 1779-51-7, Butyltriphenylphosphonium bromide 4954-12-5 6228-47-3, Propyltriphenylphosphonium bromide 7678-95-7 59077-04-2, 19-Norpregna-1,3,5(10)-trien-3-ol
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of steroid inhibitors of estrone sulfatase)

IT 4736-62-3P 6599-97-9P 13879-55-5P 13879-56-6P 31559-62-3P
34111-53-0P 57711-40-7P 64215-82-3P 99898-93-8P
120574-27-8P 120574-28-9P 123715-79-7P 137352-12-6P 206442-55-9P
208758-18-3P 208758-19-4P 208758-24-1P 208758-26-3P 208758-27-4P
208758-28-5P 208758-29-6P 208758-30-9P 208758-31-0P 208758-32-1P
208758-40-1P 208758-42-3P 208758-44-5P 208758-45-6P 208758-46-7P
208758-47-8P 208758-50-3P 208758-51-4P 208758-53-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of steroid inhibitors of estrone sulfatase)

IT 208758-49-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of steroid inhibitors of estrone sulfatase)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

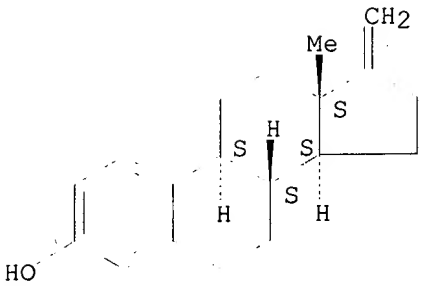
(1) Babcock; US 4297350 1981 HCAPLUS
(2) Kuehne; US 3033860 1962 HCAPLUS

IT **34111-53-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of steroid inhibitors of estrone sulfatase)

RN 34111-53-0 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-methylene- (7CI, 8CI, 9CI) (CA INDEX NAME)

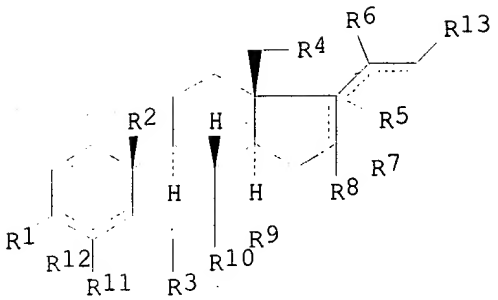
Absolute stereochemistry.



L89 ANSWER 8 OF 22 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 1998:219719 HCAPLUS
DN 128:294938
ED Entered STN: 18 Apr 1998
TI Preparation of steroids as neurochemical stimulators of the vomeronasal organ (VNO) to alleviate symptoms of anxiety
IN Jennings-White, Clive L.; Berliner, David L.; Adams, Nathan W.; Monti-Bloch, Luis
PA Pherin Pharmaceuticals, USA
SO PCT Int. Appl., 540 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM A61K031-56
CC 32-5 (Steroids)
Section cross-reference(s): 1, 2, 63
FAN.CNT 12

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9814194	A1	19980409	WO 1997-US18086	19971006 <--
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	US 6117860	A	20000912	US 1997-899094	19970723 <--
	AU 9748103	A1	19980424	AU 1997-48103	19971006 <--
PRAI	US 1996-725862	A	19961004 <--		
	US 1997-899094	A	19970723 <--		
	US 1994-286073	A2	19940804 <--		
	US 1996-625268	A2	19960329 <--		
	US 1996-686092	A2	19960723 <--		
	WO 1997-US18086	W	19971006 <--		

GI



I

AB Steroids, such as I [R1 = oxo, OH, alkoxy; R2 = alkyl, etc.; R3 = H, oxo, halo, OH, etc.; R4 - R12 = H, Me, etc.; R13 = H, Me, methylene, etc.; R2R3 = cyclic ether], were prepared for nasal administration to alleviate symptoms of anxiety. The nasally administered steroid, which is a human vomeropherin, binds to a specific neuroepithelial receptor. Thus, 3α- and 3β-pregna-4,20-dien-3-ols were prepared in 14 and 23% yields, resp., by reduction of pregna-4,20-dien-3-one using lithium trisamylborohydride in THF. Autonomic responses to stimulation of the VNO by the prepared compds. was measured.

ST steroid prepn neurochem stimulator vomeronasal organ

IT Drug delivery systems
(nasal; preparation of steroids as neurochem. stimulators of the vomeronasal organ (VNO) to alleviate symptoms of anxiety)

IT Neurohormone receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(neuroepithelial; preparation of steroids as neurochem. stimulators of the vomeronasal organ (VNO) to alleviate symptoms of anxiety)

IT Anxiolytics
(preparation of steroids as neurochem. stimulators of the vomeronasal organ (VNO) to alleviate symptoms of anxiety)

IT Nose
(vomeronasal organ; preparation of steroids as neurochem. stimulators of the vomeronasal organ (VNO) to alleviate symptoms of anxiety)

IT 846-45-7P 1150-90-9P, Estra-1,3,5(10),16-tetraen-3-ol 1224-94-8P 2118-31-2P 4075-07-4P, Androsta-4,16-dien-3-one 7628-02-6P 19865-18-0P 21321-88-0P 28336-31-4P **34111-53-0P** 35456-72-5P 35581-65-8P, Pregna-4,16-dien-3-one 55105-93-6P 65754-63-4P, Pregna-1,4,20-trien-3-one 71496-98-5P, Estra-4,16-dien-3-one 71683-67-5P 77257-06-8P 86306-95-8P 97560-70-8P, 19-Norpregna-1,3,5(10),20-tetraen-3-ol 99898-93-8P, 19-Norpregna-1,3,5(10),17(20),20-pentaen-3-ol 105644-55-1P 105663-60-3P 161061-73-0P 161061-86-5P 161061-95-6P 161061-97-8P 161061-98-9P, Estra-5(10),16-dien-3-one 161062-00-6P 177349-45-0P 177349-47-2P 177349-58-5P, 24-Norchola-4,22-dien-3-one 177349-64-3P 177349-66-5P 177565-58-1P 177794-25-1P 177794-27-3P 177794-29-5P 177794-30-8P 177856-06-3P 177856-09-6P 177856-10-9P, Estra-1,3,5(10),7,16-pentaen-3-ol 177856-12-1P 177856-13-2P, Estra-1,3,5,7,9,16-hexaen-3-ol 177856-15-4P 177856-17-6P 177856-18-7P 178688-50-1P 178688-52-3P 186183-19-7P, 19-Norpregna-5(10),20-dien-3-one 186183-25-5P 200511-32-6P 200511-37-1P 200511-39-3P 200511-50-8P, 19,21-Dinorchola-5(10),16-dien-3-one 202718-11-4P 205994-17-8P 205994-18-9P 205994-19-0P 205994-25-8P, Androsta-3,5,16-trien-3-ol 205994-26-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of steroids as neurochem. stimulators of the vomeronasal organ (VNO) to alleviate symptoms of anxiety)

IT 472-56-0P 3091-04-1P, Pregna-5,17,20-dien-3β-ol 4350-65-6P 14508-15-7P, Pregna-4,20-dien-3-one 16377-13-2P 21321-95-9P 23062-06-8P 26400-72-6P 30505-67-0P 58594-49-3P 63014-91-5P, Androsta-4,6,16-trien-3-one 71016-68-7P 86306-63-0P 86306-96-9P 99898-92-7P, 19-Norpregna-1,3,5(10)-trien-20-yn-3-ol 161061-71-8P 161061-72-9P 161061-81-0P 161061-82-1P 161061-99-0P, Estra-4,9,16-trien-3-one 161062-01-7P 161062-02-8P 161062-04-0P, Estra-1,3,5(10),7-tetraen-3-ol 161062-05-1P 161062-09-5P 177349-46-1P 177349-48-3P, 24-Norchola-4,20(22)-diene-3,6-dione 177349-49-4P, 24-Norchola-4,20(22)-dien-3-one 177349-54-1P 177349-55-2P 177349-56-3P, Pregna-4,16-diene-3,6-dione 177349-57-4P, Pregna-4,17(20),20-triene-3,6-dione 177349-59-6P 177349-60-9P, 24-Norchola-4,22-diene-3,6-dione 177349-61-0P 177349-63-2P 177349-65-4P 177349-67-6P 177349-68-7P 177349-69-8P 177349-72-3P, Pregna-1,4,20-trien-3-ol 177349-73-4P, Pregna-4,20-diene-3,6-dione 177695-29-3P 177794-21-7P 177794-22-8P 177794-24-0P 177794-26-2P 177794-31-9P 177856-07-4P, Estra-1,3,5(10),6,16-pentaen-3-ol 177856-08-5P 177856-11-0P 177856-14-3P 177856-16-5P 177856-19-8P 177856-20-1P 177856-21-2P 177856-22-3P 177856-23-4P 178033-52-8P, Estra-1,3,5(10),16-tetraene-3,6-diol 178033-53-9P, Estra-4,16-dien-3-ol 186183-17-5P 186183-18-6P, 19-Norpregna-1,3,5(10),16,20-pentaen-3-ol 186183-20-0P, 19-Norpregna-5(10),20-dien-3-ol 186183-21-1P 186183-22-2P, 19-Norpregna-4,9,20-trien-3-one 186183-26-6P 190596-13-5P, Estra-5(10),16-dien-3-ol 200511-34-8P 200574-68-1P, 19,21-Dinorchol-4-en-3-one 202718-04-5P 202718-08-9P 202718-10-3P 205994-20-3P 205994-21-4P 205994-22-5P 205994-23-6P 205994-27-0P 205994-28-1P 205994-29-2P 205994-34-9P 205994-66-7P 205994-68-9P, Pregna-1,5,20-trien-3-one 205994-73-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of steroids as neurochem. stimulators of the vomeronasal organ (VNO) to alleviate symptoms of anxiety)

IT 53-16-7, Estrone, reactions 53-43-0 57-63-6 58-22-0, Testosterone 145-13-1, 3β-HydroxyPregn-5-en-20-one 474-86-2, Equilin 517-09-9, Equilenin 1162-53-4 1425-10-1 2208-12-0, 6-Dehydroestrone 2857-45-6 3604-60-2 4736-62-3 13244-39-8 13258-68-9 14030-45-6 16397-00-5 17879-91-3 21321-89-1, Pregn-4-en-20-yn-3-one 33767-87-2 38388-13-5 38978-06-2 39006-59-2 57597-07-6 59452-16-3, 19,21-Dinorchola-1,3,5(10)-trien-3-ol 60149-52-2 60149-53-3, 19-Norpregna-4,20-dien-3-one 71716-18-2 93998-04-0 120574-28-9 161061-70-7 177349-71-2 177349-74-5 178603-56-0 205994-49-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of steroids as neurochem. stimulators of the vomeronasal organ (VNO) to alleviate symptoms of anxiety)

IT 34988-34-6P 205994-39-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of steroids as neurochem. stimulators of the vomeronasal organ (VNO) to alleviate symptoms of anxiety)

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

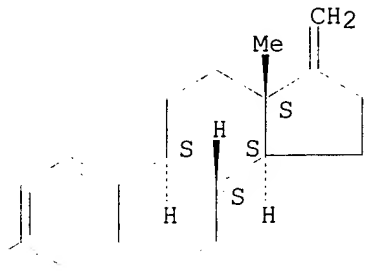
(1) Berliner; US 5563131 A 1996 HCAPLUS

IT **34111-53-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of steroids as neurochem. stimulators of the vomeronasal organ (VNO) to alleviate symptoms of anxiety)

RN 34111-53-0 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-methylene- (7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



L89 ANSWER 9 OF 22 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 1998:87643 HCAPLUS
DN 128:154277
ED Entered STN: 14 Feb 1998
TI Preparation of steroids as neurochemical stimulators of the VNO to alleviate symptoms of PMS and anxiety
IN Jennings-White, Clive L.; Berliner, David L.; Adams, Nathan W.; Bloch-Monti, Luis
PA Pherin Corp., USA
SO PCT Int. Appl., 551 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM A61K051-04
ICS C07J071-00
CC 32-5 (Steroids)
Section cross-reference(s): 2, 63
FAN.CNT 12

	PATENT NO.	KIND	DATE		APPLICATION NO.	DATE	
PI	WO 9803207	A1	19980129		WO 1997-US13035	19970723	<--
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM						
	RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG						
	US 6057439	A	20000502		US 1996-686092	19960723	<--
	AU 9739637	A1	19980210		AU 1997-39637	19970723	<--
	AU 726625	B2	20001116				
	EP 914165	A1	19990512		EP 1997-937019	19970723	<--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO						
	BR 9711812	A	19990824		BR 1997-11812	19970723	<--
	NZ 333671	A	20000728		NZ 1997-333671	19970723	<--
	JP 2000513000	T2	20001003		JP 1998-507230	19970723	<--
	NO 9900305	A	19990322		NO 1999-305	19990122	<--
	MX 9900885	A	20000331		MX 1999-885	19990122	<--
PRAI	US 1996-686092	A	19960723	<--			
	US 1996-725862	A	19961004	<--			
	US 1994-286073	A2	19940804	<--			
	US 1996-625268	A2	19960329	<--			
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OS MARPAT 128:154277

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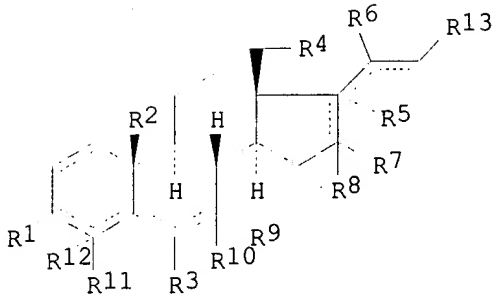

I

AB Compds. such as formula I [R1 = oxo, (substituted) OH; R2 = alkyl, etc.; R3 = H, oxo, halo, OH, etc.; R4-R12 = H, halo, Me; R13 = H, Me, methylene, etc.; R2R3 = cyclic ether] are prepared The invention relates to a method of alleviating the symptoms of PMS and anxiety. The method comprises nasally administering a steroid which is a human vomeropherin, such that the vomeropherin binds to a specific neuroepithelial receptor. The steroid or steroids is/are preferably administered in the form of a pharmaceutical composition containing one or more pharmaceutically acceptable carriers.

ST steroid prepn neurochem stimulator vomeronasal organ

IT Drug delivery systems
(nasal; preparation of steroids as neurochem. stimulators of the vomeronasal organ)

IT Receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(neuroepithelial; preparation of steroids as neurochem. stimulators of the vomeronasal organ)

IT Ovarian cycle
(premenstrual syndrome; preparation of steroids as neurochem. stimulators of the vomeronasal organ)

IT Anxiolytics
(preparation of steroids as neurochem. stimulators of the vomeronasal organ)

IT Nose
(vomeronasal organ; preparation of steroids as neurochem. stimulators of the vomeronasal organ)

IT 1150-90-9P, Estra-1,3,5(10),16-tetraen-3-ol 4075-07-4P, Androsta-4,16-dien-3-one 4736-62-3P 14508-15-7P, Pregna-4,20-dien-3-one 28336-31-4P 65754-63-4P, Pregna-1,4,20-trien-3-one 71496-98-5P, Estra-4,16-dien-3-one 161061-70-7P 161061-73-0P 161061-81-0P 161061-82-1P 161061-97-8P 177349-47-2P 177349-52-9P 177349-58-5P, 24-Norchola-4,22-dien-3-one 177856-07-4P, Estra-1,3,5(10),6,16-pentaen-3-ol 178688-52-3P 200511-50-8P, 19,21-Dinorchola-5(10),16-dien-3-one 202718-11-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of steroids as neurochem. stimulators of the vomeronasal organ)

IT 53-63-4P, Estra-1,3,5(10)-trien-3-ol 472-56-0P 2872-90-4P, Androst-4-en-3-one 16377-13-2P 21321-95-9P 23062-06-8P 26400-72-6P 30505-67-0P 58594-49-3P 63014-91-5P, Androsta-4,6,16-trien-3-one 86306-63-0P 86306-96-9P 99898-92-7P, 19-Norpregna-1,3,5(10)-trien-20-yn-3-ol 114611-55-1P, Androsta-4,16-diene-3,6-dione 161061-71-8P 161061-72-9P 161061-83-2P 161061-84-3P 161061-99-0P, Estra-4,9,16-trien-3-one 161062-01-7P 161062-02-8P 161062-04-0P,

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202718-08-9P 202718-09-0P 202718-10-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of steroids as neurochem. stimulators of the vomeronasal organ)

IT 53-16-7, Estrone, reactions 53-43-0, Dehydroepiandrosterone 57-63-6, Ethinylestradiol 58-22-0, Testosterone 145-13-1 434-22-0, 19-Nortestosterone 474-86-2, Equilin 517-09-9, Equilenin 1162-53-4 1434-85-1 2118-31-2 2208-12-0, 6-Dehydroestrone 2857-45-6 3604-60-2 13244-39-8 13258-68-9 14030-45-6 16397-00-5 17879-91-3 21321-88-0 21321-89-1, Pregn-4-en-20-yn-3-one 35581-65-8, Pregna-4,16-dien-3-one 38388-13-5 38978-06-2 39006-59-2 57597-07-6 60149-52-2 60149-53-3, 19-Norpregna-4,20-dien-3-one 63015-08-7, Androsta-1,4,16-trien-3-one 71716-18-2 93998-04-0 120574-28-9 177349-70-1 177349-71-2 177565-58-1 177794-28-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of steroids as neurochem. stimulators of the vomeronasal organ)

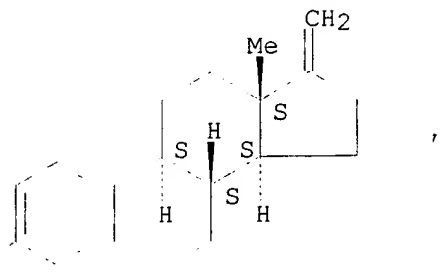
IT 846-45-7P 1224-94-8P 7628-02-6P, Estrone hydrazone 19865-18-0P 33767-87-2P **34111-53-0P** 34988-34-6P 35456-72-5P 55105-93-6P 59452-16-3P, 19,21-Dinorchola-1,3,5(10)-trien-3-ol 71683-67-5P 77257-06-8P 86306-95-8P 97560-70-8P, 19-Norpregna-1,3,5(10),20-tetraen-3-ol 99898-93-8P 103614-70-6P, Androsta-5,16-dien-3-one 105644-55-1P 105663-60-3P 161061-86-5P 161061-93-4P 161061-95-6P 161061-98-9P, Estra-5(10),16-dien-3-one 161062-00-6P 177349-45-0P 177349-50-7P 177349-51-8P 177349-64-3P 177349-66-5P 177349-74-5P 177794-25-1P 177794-29-5P 177794-30-8P 177856-06-3P 177856-09-6P 177856-10-9P, Estra-1,3,5(10),7,16-pentaen-3-ol 177856-12-1P 177856-13-2P, Estra-1,3,5,7,9,16-hexaen-3-ol 177856-15-4P 177856-17-6P 177856-18-7P 178688-50-1P 186183-19-7P, 19-Norpregna-5(10),20-dien-3-one 186183-25-5P 200511-32-6P 200511-37-1P 200511-39-3P 202718-05-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of steroids as neurochem. stimulators of the vomeronasal organ)

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Gee; US 5208227 1993 HCAPLUS

IT **34111-53-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of steroids as neurochem. stimulators of the vomeronasal organ)

RN 34111-53-0 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methylene- (7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



L89 ANSWER 10 OF 22 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 1997:672282 HCAPLUS
DN 127:293468
ED Entered STN: 23 Oct 1997
TI Preparation of steroids as neurochemical initiators of change in human blood levels of LH or FSH
IN Jennings-White, Clive L.; Berliner, David L.; Adams, Nathan W.
PA Pherin Corp., USA
SO PCT Int. Appl., 498 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM A61K031-56
CC 32-5 (Steroids)
Section cross-reference(s): 2, 63
FAN.CNT 12

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9736596	A1	19971009	WO 1997-US6061	19970328 <--
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	RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
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	AU 735804	B2	20010712		
	EP 891188	A1	19990120	EP 1997-918578	19970328 <--
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	JP 2000504025	T2	20000404	JP 1997-535629	19970328 <--
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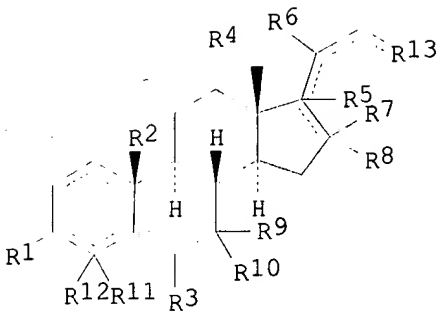
	US 1994-286073	A2	19940804 <--		
	WO 1997-US6061	W	19970328 <--		

GI



I

AB The invention relates to a method of altering the blood levels of LH or FSH in an individual. Steroids of formula I [R1 = oxo, OH, OAc, O2CEt, methoxy, etc.; R2 = Me, HOCH2, acyloxymethyl, alkyl, etc.; R3 = H, oxo, halo, OH, alkoxy, acyloxy; R4-R12 = H, halo, Me, halomethyl; R13 = H, Me, methylene, Et, ethenyl, acetylenyl, etc.], and others are prepared The method comprises nasally administering a steroid which is a human vomeropherin, such that the vomeropherin binds to a specific neuroepithelial receptor. The steroid or steroids is/are preferably administered in the form of a pharmaceutical composition containing one or more pharmaceutically acceptable carriers. Thus, 1,3,5(10),16-estratetraen-3-ol is prepared from estrone via hydrazone formation and reduction 1,3,5(10),16-Estratetraen-3-ol is shown to have autonomic activity.

ST FSH regulation steroid prepn; testosterone regulation steroid prepn; vomeronasal organ FSH regulation steroid prepn; neuroepithelial receptor FSH regulation steroid prepn; LH regulation steroid prepn

IT Drug delivery systems
(nasal; preparation of steroids as neurochem. initiators of change in human blood levels of LH or FSH)

IT Receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(neuroepithelial; preparation of steroids as neurochem. initiators of change in human blood levels of LH or FSH)

IT Nose
(neuroepithelium; preparation of steroids as neurochem. initiators of change in human blood levels of LH or FSH)

IT Nose
(vomeronasal organ; preparation of steroids as neurochem. initiators of change in human blood levels of LH or FSH)

IT 28336-31-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of steroids as neurochem. initiators of change in human blood levels of LH or FSH)

IT 1150-90-9P, Estra-1,3,5(10),16-tetraen-3-ol 4075-07-4P, Androsta-4,16-dien-3-one 65754-63-4P, Pregna-1,4,20-trien-3-one 161061-73-0P 177349-45-0P 177349-47-2P 177349-52-9P 177349-74-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of steroids as neurochem. initiators of change in human blood levels of LH or FSH)

IT 2118-31-2
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)

(preparation of steroids as neurochem. initiators of change in human blood levels of LH or FSH)

IT 53-63-4P, Estra-1,3,5(10)-trien-3-ol 2872-90-4P, Androst-4-en-3-one 21321-95-9P 23062-06-8P 26400-72-6P 30505-67-0P 58594-49-3P 63014-91-5P, Androsta-4,6,16-trien-3-one 86306-63-0P 86306-96-9P 114611-55-1P, Androsta-4,16-diene-3,6-dione 120476-05-3P 161061-71-8P 161061-72-9P 161061-81-0P 161061-82-1P 161061-83-2P 161061-84-3P 161061-99-0P, Estra-4,9,16-trien-3-one 161062-01-7P 161062-02-8P 161062-04-0P, Estra-1,3,5(10),7-tetraen-3-ol 161062-05-1P 161062-06-2P, Estra-1,3,5(10),6-tetraen-3-ol 161062-08-4P 161062-09-5P 177349-46-1P 177349-48-3P, 24-Norchola-4,20(22)-diene-3,6-dione 177349-49-4P, 24-Norchola-4,20(22)-dien-3-one 177349-53-0P 177349-54-1P 177349-55-2P 177349-56-3P, Pregna-4,16-diene-3,6-dione 177349-57-4P, Pregna-4,17(20),20-triene-3,6-dione 177349-59-6P 177349-60-9P, 24-Norchola-4,22-diene-3,6-dione 177349-61-0P 177349-62-1P 177349-63-2P 177349-65-4P 177349-67-6P 177349-68-7P 177349-69-8P 177349-72-3P, Pregna-1,4,20-trien-3-ol 177349-73-4P, Pregna-4,20-diene-3,6-dione 177695-29-3P 177794-21-7P 177794-22-8P 177794-23-9P 177794-24-0P 177794-26-2P 177794-27-3P 177794-31-9P 177794-32-0P 177856-05-2P 177856-08-5P 177856-11-0P 177856-14-3P 177856-16-5P 177856-19-8P 177856-20-1P 177856-21-2P 177856-22-3P 177856-23-4P 178033-52-8P, Estra-1,3,5(10),16-tetraene-3,6-diol 178033-53-9P, Estra-4,16-dien-3-ol 186183-17-5P 186183-18-6P 186183-20-0P, 19-Norpregna-5(10),20-dien-3-ol 186183-21-1P 186183-22-2P, 19-Norpregna-4,9,20-trien-3-one 186183-26-6P 186183-27-7P 186183-28-8P 186183-29-9P 197094-33-0P 197094-34-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of steroids as neurochem. initiators of change in human blood levels of LH or FSH)

IT 9002-67-9, Luteinizing hormone 9002-68-0, Follicle stimulating hormone
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(preparation of steroids as neurochem. initiators of change in human blood levels of LH or FSH)

IT 58-22-0, Testosterone
RL: BPR (Biological process); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); PROC (Process); RACT (Reactant or reagent)
(preparation of steroids as neurochem. initiators of change in human blood levels of LH or FSH)

IT 53-16-7, Estrone, reactions 53-43-0, Dehydroepiandrosterone 57-63-6 145-13-1 434-22-0, 19-Nortestosterone 474-86-2, Equilin 517-09-9, Equilenin 1162-53-4 2208-12-0, 6-Dehydroestrone 2857-45-6 3604-60-2 6228-47-3, Propyltriphenylphosphonium bromide 13244-39-8 13258-68-9 14030-45-6 14508-15-7, Pregna-4,20-dien-3-one 17879-91-3 21321-88-0, Pregna-5,20-dien-3β-ol 21321-89-1, Pregn-4-en-20-yn-3-one 38388-13-5 38978-06-2 39006-59-2 57597-07-6 60149-52-2 60149-53-3, 19-Norpregna-4,20-dien-3-one 63015-08-7, Androsta-1,4,16-trien-3-one 71716-18-2 93998-04-0 177349-70-1 177349-71-2 177565-58-1 177794-28-4 178603-56-0 190596-19-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of steroids as neurochem. initiators of change in human blood levels of LH or FSH)

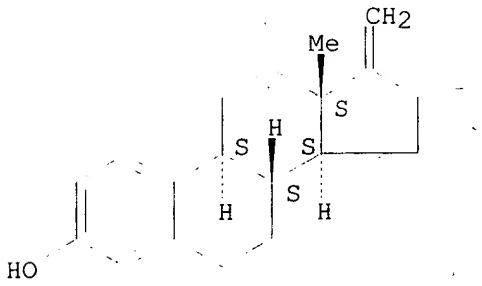
IT 846-45-7P 1224-94-8P 19865-18-0P **34111-53-0P** 34988-34-6P 35456-72-5P 55105-93-6P 71496-98-5P, Estra-4,16-dien-3-one 77257-06-8P 86306-95-8P 97560-70-8P, 19-Norpregna-1,3,5(10),20-tetraen-3-ol 99898-92-7P, 19-Norpregna-1,3,5(10)-trien-20-yn-3-ol 99898-93-8P 103614-70-6P, Androsta-5,16-dien-3-one 161061-70-7P 161061-86-5P 161061-93-4P 161061-95-6P 161061-97-8P 161061-98-9P, Estra-5(10),16-dien-3-one 161062-00-6P 177349-50-7P 177349-51-8P 177349-58-5P, 24-Norchola-4,22-dien-3-one 177349-64-3P 177349-66-5P

177794-25-1P 177794-29-5P 177794-30-8P 177856-06-3P 177856-07-4P,
Estra-1,3,5(10),6,16-pentaen-3-ol 177856-09-6P 177856-10-9P,
Estra-1,3,5(10),7,16-pentaen-3-ol 177856-12-1P 177856-13-2P,
Estra-1,3,5,7,9,16-hexaen-3-ol 177856-15-4P 177856-17-6P
177856-18-7P 186183-19-7P, 19-Norpregna-5(10),20-dien-3-one
186183-25-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of steroids as neurochem. initiators of change in human blood levels of LH or FSH)

IT **34111-53-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of steroids as neurochem. initiators of change in human blood levels of LH or FSH)

RN 34111-53-0 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methylene- (7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



L89 ANSWER 11 OF 22 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 1997:394816 HCAPLUS
DN 127:17859
ED Entered STN: 26 Jun 1997
TI Preparation of estrenes for inducing hypothalamic effects
IN Berliner, David L.; Adams, Nathan W.; Jennings-White, Clive L.
PA Pherin Corporation, USA
SO U.S., 63 pp., Division of U.S. Ser. No. 316,050.
CODEN: USXXAM
DT Patent
LA English
IC ICM C07J013-00
NCL 552530000
CC 32-3 (Steroids)
Section cross-reference(s): 1
FAN.CNT 7

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PI	US 5633392	A	19970527		US 1995-454917	19950531	<--
	US 5783571	A	19980721		US 1993-127980	19930928	<--
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PRAI	US 1991-638743	B2	19910107	<--			
	US 1991-707862	B2	19910531	<--			
	US 1992-903525	B2	19920624	<--			
	US 1993-127980	A2	19930928	<--			

US 1994-316050	A3	19940929	<--
US 1993-127908	B2	19930928	<--
EP 1995-935237	A3	19950929	<--
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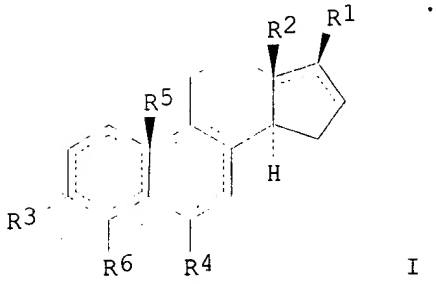
OS MARPAT 127:17859

GI



I

AB The invention relates to estrene steroids, which bind to neuroepithelial receptors. Title compds. I [R1 = CH2, Me; R2 = null, H, Me; R3 = oxo, OH, alkoxy, acyloxy, benzoyl, etc.; R4 = H, OH, alkoxy, acyloxy, oxo, halo; R5 = null, H, OH, alkoxy, acyloxy; R6 = H, halo; with provisos] are prepared and tested for their effect on olfactory receptors. Refluxing a mixture of estrone, p-toluenesulfonylhydrazide in methanol for 20 h gave estrone p-toluenesulfonylhydrazone, which was treated with BuLi in hexane-THF with ice cooling to give the title compound estra-1,3,5(10),16-tetraen-3-ol. Stimulation on human vomeronasal organ by this gave a local elec. potential response of ca. 22 mV-seconds vs. ca. 8 mV-seconds for androstadien-3-one.

ST estrene prepn hypothalamic effect

IT Brain
(hypothalamus; preparation of estrenes for inducing hypothalamic effects)

IT Drug delivery systems
(nasal; preparation of estrenes for inducing hypothalamic effects)

IT Anxiolytics
Odor and Odorous substances
(preparation of estrenes for inducing hypothalamic effects)

IT Steroids, preparation
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of estrenes for inducing hypothalamic effects)

IT Sensory receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(preparation of estrenes for inducing hypothalamic effects)

IT 1150-90-9P, Estra-1,3,5(10),16-tetraen-3-ol **34111-53-0P**
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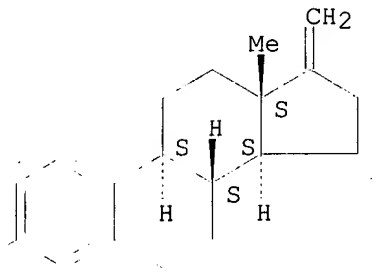
177856-06-3P 177856-09-6P 177856-10-9P, Estra-1,3,5(10),7,16-pentaen-3-ol 177856-13-2P, Estra-1,3,5,7,9,16-hexaen-3-ol 177856-15-4P
177856-17-6P 177856-18-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT

(Reactant or reagent); USES (Uses)
(preparation of estrenes for inducing hypothalamic effects)
IT 161061-99-0P, Estra-4,9,16-trien-3-one 161062-02-8P 161062-04-0P, Estra-1,3,5(10),7-tetraen-3-ol 161062-05-1P 161062-06-2P, Estra-1,3,5(10),6-tetraen-3-ol 177856-07-4P, Estra-1,3,5(10),6,16-pentaen-3-ol 177856-08-5P 177856-11-0P 177856-12-1P 177856-14-3P 177856-16-5P 177856-19-8P 177856-20-1P 177856-21-2P 177856-22-3P 177856-23-4P 178033-52-8P, Estra-1,3,5(10),16-tetraene-3,6-diol 178033-53-9P, Estra-4,16-dien-3-ol 190596-13-5P, Estra-5(10),16-dien-3-ol 190596-16-8P 190596-17-9P 190596-18-0P, Estra-4,8,16-trien-3-one
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of estrenes for inducing hypothalamic effects)
IT 53-16-7, Estrone, reactions 434-22-0, 19-Nortestosterone 474-86-2, Equilin 517-09-9, Equilenin 1576-35-8, p-Toluenesulfonylhydrazide 1779-49-3, Triphenylmethylphosphonium bromide 2208-12-0, 6-Dehydroestrone 28336-31-4 93998-04-0 190596-19-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of estrenes for inducing hypothalamic effects)
IT 1425-10-1P, 19-Nortestosterone acetate 55105-93-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of estrenes for inducing hypothalamic effects)
IT **34111-53-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of estrenes for inducing hypothalamic effects)
RN 34111-53-0 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methylene- (7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



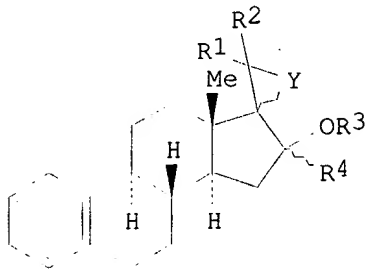
L89 ANSWER 12 OF 22 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 1997:244398 HCAPLUS
DN 126:225448
ED Entered STN: 16 Apr 1997
TI Novel estrogens for treating autoimmune diseases
IN Brattsand, Ralph; Holmdahl, Rikard; Jansson, Liselotte; Loncar, Marjana; Pettersson, Lars
PA Astra Aktiebolag, Swed.; Brattsand, Ralph; Holmdahl, Rikard; Jansson, Liselotte; Loncar, Marjana; Pettersson, Lars
SO PCT Int. Appl., 53 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07J053-00
CC 32-3 (Steroids)

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9708188	A1	19970306	WO 1996-SE1028	19960820 <--
	W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM				
	CA 2228803	AA	19970306	CA 1996-2228803	19960820 <--
	AU 9668405	A1	19970319	AU 1996-68405	19960820 <--
	EP 847399	A1	19980617	EP 1996-928771	19960820 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI				
	JP 11511457	T2	19991005	JP 1997-510174	19960820 <--
	US 6043236	A	20000328	US 1997-817683	19970423 <--
PRAI	SE 1995-2921	A	19950823 <--		
	WO 1996-SE1028	W	19960820 <--		

OS MARPAT 126:225448

GI



RO I

AB Estratrienes I [R = H, alkyl, cycloalkyl, acyl, alkoxycarbonyl, aralkoxycarbonyl, protective group; R1, R2 = H, Me, Et, halogen; R3 = H, acyl, alkoxycarbonyl, aralkoxycarbonyl; R4 = H, Me, Et; Y = CH2, bond] were prepared Thus, estrone was converted to its 3-dimethylthexyl ether which was treated with EtPPh3+ Br-, followed by SeO2-Me3COOH oxidation and desilylation to give (17E)-3,16α-dihydroxy-19-norpregna-1,3,5(10),17(20)-tetraene. I show very low sex hormone side effects while retaining their antiinflammatory and immunosuppressant activity.

ST estratriene deriv prepn antiinflammatory immunosuppressant

IT Anti-inflammatory agents
Immunosuppressants
(preparation of estratriene derivs. as inflammation inhibitors and immunosuppressants)

IT Estrogens
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of estratriene derivs. as inflammation inhibitors and immunosuppressants)

IT 50-27-1, Estriol 53-16-7, Estrone, reactions 867-13-0, Triethyl phosphonoacetate **34111-53-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of estratriene derivs. as inflammation inhibitors and immunosuppressants)

IT 188291-18-1P 188291-19-2P 188291-20-5P 188291-21-6P 188291-22-7P

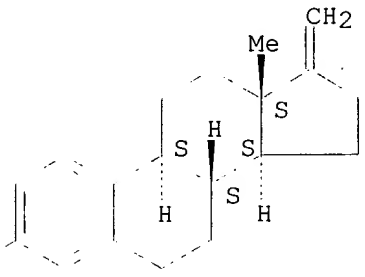
188291-23-8P 188291-27-2P 188291-30-7P 188291-31-8P 188291-33-0P
188291-34-1P 188291-36-3P 188291-37-4P 188291-38-5P 188291-39-6P
188291-42-1P 188291-43-2P 188291-44-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of estratriene derivs. as inflammation inhibitors and immunosuppressants)

IT 70574-32-2P 188291-24-9P 188291-25-0P 188291-26-1P 188291-28-3P
188291-29-4P 188291-32-9P 188291-35-2P 188291-40-9P 188291-41-0P
188291-45-4P 188291-48-7P 188291-49-8P 188291-50-1P 188291-51-2P
188291-52-3P 188291-53-4P 188291-54-5P 188291-55-6P 188291-56-7P
188291-57-8P 188291-58-9P 188291-60-3P 188291-62-5P 188291-63-6P
188291-65-8P 188291-67-0P 188291-70-5P 188291-72-7P 188291-74-9P
188291-76-1P 188291-79-4P 188291-80-7P 188291-81-8P 188291-83-0P
188291-86-3P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of estratriene derivs. as inflammation inhibitors and immunosuppressants)

IT **34111-53-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of estratriene derivs. as inflammation inhibitors and immunosuppressants)

RN 34111-53-0 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methylene- (7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



L89 ANSWER 13 OF 22 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 1996:369795 HCAPLUS
DN 125:58846
ED Entered STN: 27 Jun 1996
TI Novel estrenes for inducing hypothalamic effects
IN Berliner, David L.; Adams, Nathan W.; Jennings-White, Clive L.
PA Pherin Corporation, USA
SO PCT Int. Appl., 137 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07J001-00
ICS C07J003-00; C07J031-00; C07J053-00
CC 32-3 (Steroids)
Section cross-reference(s): 1
FAN.CNT 7

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9610032	A1	19960404	WO 1995-US12542	19950929 <--

W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ,

TM, TT
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

NZ 333837	A	20000526	NZ 1995-333837	19950529	<--	
CA 2199044	AA	19960404	CA 1995-2199044	19950929	<--	
AU 9537331	A1	19960419	AU 1995-37331	19950929	<--	
AU 705422	B2	19990520				
EP 783513	A1	19970716	EP 1995-935237	19950929	<--	
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE						
CN 1167489	A	19971210	CN 1995-196518	19950929	<--	
HU 76856	A2	19971229	HU 1997-1508	19950929	<--	
BR 9509098	A	19980714	BR 1995-9098	19950929	<--	
JP 10509423	T2	19980914	JP 1995-512067	19950929	<--	
EP 924219	A2	19990623	EP 1998-203950	19950929	<--	
EP 924219	A3	20020123				
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV						
RU 2160279	C2	20001210	RU 1997-107609	19950929	<--	
NO 9701417	A	19970523	NO 1997-1417	19970325	<--	
FI 9701315	A	19970327	FI 1997-1315	19970327	<--	
PRAI US 1994-316050	A	19940929	<--			
EP 1995-935237	A3	19950929	<--			
NZ 1995-294510	A1	19950929	<--			
WO 1995-US12542	W	19950929	<--			

OS MARPAT 125:58846

AB The invention relates to estrene steroid, which bind to neuroepithelial receptors. Thus,estrone is converted to its tosylhydrazone which is subjected to elimination reaction to give 1,3,5(10),16-estratetraen-3-ol (I). I elicits a response in the vomeronasal organ that is stronger in males than females.

ST estrene deriv prepn hypothalamus

IT Hypothalamus
(preparation of estrenes for inducing hypothalamic effects)

IT Steroids, preparation
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of estrenes for inducing hypothalamic effects)

IT 28336-31-4
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(preparation of estrenes for inducing hypothalamic effects)

IT 1150-90-9P, Estra-1,3,5(10),16-tetraen-3-ol 161061-73-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of estrenes for inducing hypothalamic effects)

IT 161062-09-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of estrenes for inducing hypothalamic effects)

IT 50-27-1 58-22-0 1224-94-8 4075-07-4, Androsta-4,16-dien-3-one
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of estrenes for inducing hypothalamic effects)

IT 53-16-7, Estrone, reactions 434-22-0, 19-Nortestosterone 474-86-2, Equilin 517-09-9, Equilenin 2208-12-0, 6-Dehydroestrone 33767-87-2 93998-04-0 161061-98-9, Estra-5(10),16-dien-3-one
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of estrenes for inducing hypothalamic effects)

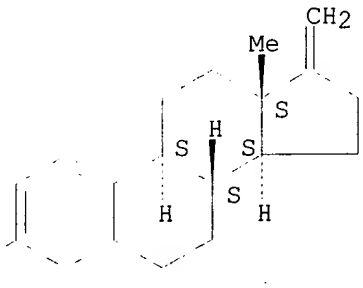
IT **34111-53-0P** 35456-72-5P 55105-93-6P 71496-98-5P, Estra-4,16-dien-3-one 77257-06-8P 86306-95-8P 161061-97-8P 161062-00-6P 177856-06-3P 177856-07-4P, Estra-1,3,5(10),6,16-pentaen-3-ol 177856-09-6P 177856-10-9P, Estra-1,3,5(10),7,16-pentaen-3-ol 177856-12-1P 177856-15-4P 177856-17-6P 177856-18-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of estrenes for inducing hypothalamic effects)

IT 58594-49-3P 86306-96-9P 161061-99-0P, Estra-4,9,16-trien-3-one 161062-01-7P 161062-02-8P 161062-03-9P 161062-04-0P, Estra-1,3,5(10),7-tetraen-3-ol 161062-05-1P 161062-06-2P, Estra-1,3,5(10),6-tetraen-3-ol 161062-07-3P 161062-08-4P 177856-05-2P 177856-08-5P 177856-11-0P 177856-13-2P, Estra-1,3,5,7,9,16-hexaen-3-ol 177856-14-3P 177856-16-5P 177856-19-8P 177856-20-1P 177856-21-2P 177856-22-3P 177856-23-4P 177856-24-5P 178033-52-8P, Estra-1,3,5(10),16-tetraene-3,6-diol 178033-53-9P, Estra-4,16-dien-3-ol
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of estrenes for inducing hypothalamic effects)

IT **34111-53-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of estrenes for inducing hypothalamic effects)

RN 34111-53-0 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methylene- (7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



L89 ANSWER 14 OF 22 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 1992:626505 HCAPLUS
DN 117:226505
ED Entered STN: 13 Dec 1992
TI Synthesis and characterization of estrogen 2,3- and 3,4-quinones. Comparison of DNA adducts formed by the quinones versus horseradish peroxidase-activated catechol estrogens
AU Dwivedy, I.; Devanesan, P.; Cremonesi, P.; Rogan, E.; Cavalieri, E.
CS Med. Cent., Univ. Nebraska, Omaha, NE, 68198-6805, USA
SO Chemical Research in Toxicology (**1992**), 5(6), 828-33
CODEN: CRTOEC; ISSN: 0893-228X
DT Journal
LA English
CC 2-4 (Mammalian Hormones)
Section cross-reference(s): 32
AB Catechol estrogens (CE) are among the major metabolites of estrone (E1) and 17β-estradiol (E2). Oxidation of these metabolites to semiquinones and quinones could generate ultimate carcinogenic froms of E1 and E2. The 2,3- and 3,4-quinones of E1 and E2 were synthesized by MnO2 oxidation of the corresponding CE. Characterization of these compds. was accomplished by UV, NMR, and mass spectrometry. The relative stability of these compds.

was determined in DMSO/H2O (2:1) at room temperature, and the 3,4-quinones were more
stable than the 2,3-quinones. The four quinones directly reacted with calf thymus DNA to form DNA adducts analyzed by the 32P-postlabeling method. The adducts were compared to those formed when the corresponding CE were activated by horseradish peroxidase (HRP) to bind to DNA. The E1- and E2-2,3-quinones formed much higher levels of DNA adducts than the corresponding 3,4-quinones. In addition, many of the adducts (70-90%) formed by the E1- and E2-2,3-quinones appeared to be the same as those formed by activation of 2-OHE1 or 2-OHE2 by HRP to bind to DNA. Little overlap was observed between the adducts formed by E1- and E2-3,4-quinones and HRP-activated 4-OHE1 and 4-OHE2. Thus, semiquinones and/or quinones are ultimate reactive intermediates in the peroxidative activation of catechol estrogens.

ST catechol estrogen peroxidase quinone; DNA adduct estrogen quinone peroxidase; estradiol quinone peroxidase hydroxyestradiol DNA; estrone quinone peroxidase hydroxyestrone DNA

IT Estrogens
RL: SPN (Synthetic preparation); PREP (Preparation)
(quinones, preparation and DNA adduct formation by, peroxidase-activated catechol estrogen in relation to)

IT Deoxyribonucleic acids
RL: BIOL (Biological study)
(adducts, with estrogen quinones, catechol estrogen activation by peroxidase in relation to)

IT Estrogens
RL: BIOL (Biological study)
(hydroxy, activation of, by peroxidase, quinone formation in, DNA adducts in relation to)

IT **7291-57-8** 144082-85-9
RL: BIOL (Biological study)
(C3-deacetylation and demethylation of)

IT 9003-99-0, Peroxidase
RL: BIOL (Biological study)
(catechol estrogen activation by, quinone formation in, DNA adducts in relation to)

IT 83649-26-7 144072-46-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(deacetylation and demethylation of)

IT 40551-33-5D, Estra-1(10),4-diene-2,3,17-trione, DNA adducts 40551-34-6D, Estra-1,5(10)-diene-3,4,17-trione, DNA adducts 42261-16-5D, DNA adducts 144082-88-2D, DNA adducts
RL: FORM (Formation, nonpreparative)
(formation of, catechol estrogen activation by peroxidase in relation to)

IT 23463-05-0P 144082-86-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acid hydrolysis of)

IT 362-05-0P, 2-Hydroxyestradiol 362-06-1P, 2-Hydroxyestrone 3131-23-5P, 4-Hydroxyestrone 5976-61-4P, 4-Hydroxyestradiol
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oxidation of)

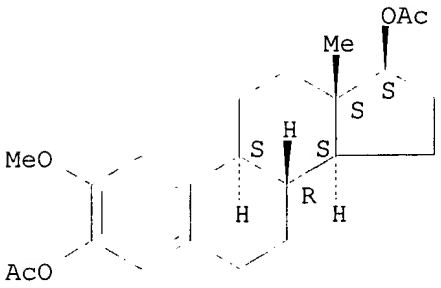
IT 40551-33-5P, Estra-1(10),4-diene-2,3,17-trione 40551-34-6P, Estra-1,5(10)-diene-3,4,17-trione 42261-16-5P 144082-88-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with DNA)

IT 144082-87-1P 144082-89-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT **7291-57-8**

RL: BIOL (Biological study)
(C3-deacetylation and demethylation of)
RN 7291-57-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-, diacetate, (17β)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



L89 ANSWER 15 OF 22 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 1990:173065 HCAPLUS
DN 112:173065
ED Entered STN: 12 May 1990
TI Preparation of 17-methylenestratrienes as contraceptives and drugs for treatment of climacteric disorders
IN Jungblut, Peter; Wiechert, Rudolf; Bittler, Dieter
PA Schering A.-G., Fed. Rep. Ger.
SO Ger. Offen., 4 pp.
CODEN: GWXXBX
DT Patent
LA German
IC ICM A61K031-57
ICS A61K031-56; C07J003-00; C07J007-00
ICA A61K009-06; A61K009-08; A61K009-20; A61K009-50; C12Q001-00
CC 2-3 (Mammalian Hormones)
Section cross-reference(s): 32
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	DE 3741801	A1	19890615	DE 1987-3741801	19871207	<--
	EP 320437	A2	19890614	EP 1988-730273	19881205	<--
	EP 320437	A3	19910731			
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE					
	CA 1329770	A1	19940524	CA 1988-585132	19881206	<--
	AU 8826653	A1	19890608	AU 1988-26653	19881207	<--
	AU 621844	B2	19920326			
	JP 01197438	A2	19890809	JP 1988-307973	19881207	<--
	US 4977147	A	19901211	US 1988-280803	19881207	<--
PRAI	DE 1987-3741801		19871207	<--		

OS CASREACT 112:173065; MARPAT 112:173065
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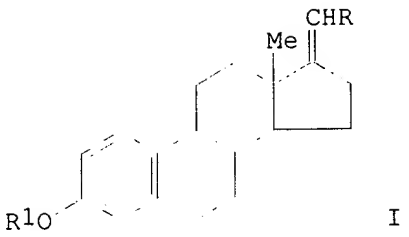


I

AB The 17-methylenestratrienes I (R = H, Me; R1 = H, Me, acyl, tetrahydropyranyl) are prepared as contraceptives, drugs for the treatment of hormone-dependent tumors, and drugs for the treatment of climacteric disorders. Compared to estrones, I show less affinity to estrogen receptors and higher cell membrane and lymph vessel permeability. A suspension of MePh3PBr in dioxane was treated with a solution of BuLi in hexane, followed by the addition of 3-(tetrahydropyran-2-yloxy)-1,3,5(10) estratrien-17-one, to give 17-methylene-3-(tetrahydropyran-2-yloxy)-1,3,5(10)estratriene. This was treated with H2SO4 in MeOH, to give 17-methylene-1,3,5(10)-estratrien-3-ol (II). Pills contained II 0.050, lactose 46.450, starch 26.800, PVP 3.000 and talc 3.700 mg/each. In uterus growth tests with young rats, II showed 1/70th of the uterotropic activity of estradiol.

ST methylenestratriene prepn contraceptive anticancer; estratriene methylene contraceptive anticancer

IT Contraceptives
Neoplasm inhibitors
(methylenestratrienes)

IT Climacteric (animal)
(treatment of, with methylenestratrienes)

IT 1530-32-1 1779-49-3, Methyltriphenylphosphonium bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(Wittig reaction of, with estratrienone derivative)

IT 57711-40-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(Wittig reaction of, with ethyltriphenylphosphonium bromide)

IT 7103-48-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(Wittig reaction of, with methyltriphenylphosphonium bromide)

IT 126400-73-5P
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

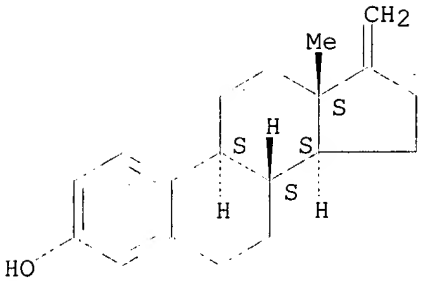
IT 4350-65-6P 32043-13-3P **34111-53-0P** 35456-72-5P 77257-06-8P
126400-71-3P 126400-72-4P
RL: PREP (Preparation)
(preparation of, as contraceptive and neoplasm inhibitor and drug for treatment of climacteric disorders)

IT **34111-53-0P**
RL: PREP (Preparation)
(preparation of, as contraceptive and neoplasm inhibitor and drug for treatment of climacteric disorders)

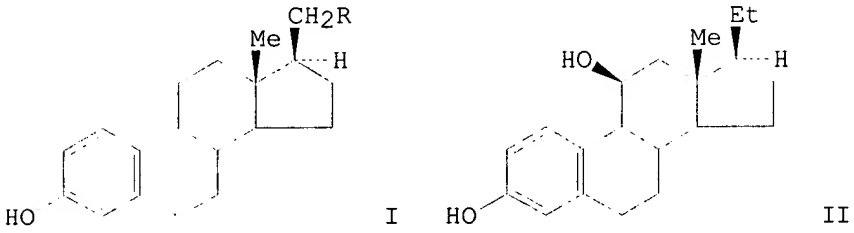
RN 34111-53-0 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-methylene- (7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



L89 ANSWER 16 OF 22 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 1989:423774 HCAPLUS
DN 111:23774
ED Entered STN: 21 Jul 1989
TI 17-Desoxy estrogen analogs
AU Peters, Richard H.; Crowe, David F.; Avery, Mitchell A.; Chong, Wesley K. M.; Tanabe, Masato
CS Bio-Org. Chem. Lab., SRI Int., Menlo Park, CA, 94025, USA
SO Journal of Medicinal Chemistry (**1989**), 32(7), 1642-52
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
CC 32-3 (Steroids)
Section cross-reference(s): 2
OS CASREACT 111:23774
GI



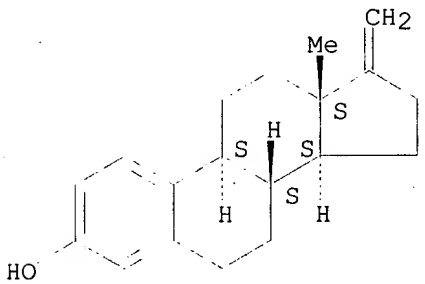
AB A series of 17-substituted 17-desoxyestratrienes, e.g. I (R = H, Me) and II, were synthesized and tested as potential postcoital antifertility agents. Estrogen-relative binding affinities were determined; in vivo assays for estrogenic and postcoital antifertility activity were conducted in rats, and selected candidate compds. were further tested for estrogenic activity in monkeys. In the rat, I (R = H, Me) and II have low estrogenic activity while retaining potent antifertility activity. Structural modifications at the outset included a variety of 17-substituents and an omission of the 17-oxygen functionality, which was previously thought to be necessary for potent activity. The 17β-Et side chain exhibited the greatest antifertility activity with the largest separation ratio to estrogenicity. Nuclear modification of 17-desoxyethylestrane derivs. at positions 7 and 11 further increased the desired separation of activity, with the 11-hydroxy moiety enhancing separation more than other features.
ST desoxy estrogen analog prepn antifertility
IT Estrogens
RL: RCT (Reactant); RACT (Reactant or reagent)
(17-substituted deoxyestratrienes as)
IT Molecular structure-biological activity relationship
(antifertility, 17-substituted deoxyestratrienes)

IT Molecular structure-biological activity relationship
(estrogenic, 17-substituted deoxyestratrienes)
IT Fertility
(inhibitors, 17-substituted deoxyestratrienes as)
IT 2344-80-1, (Chloromethyl)trimethylsilane
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of, with norpregnatrienone derivative)
IT 53-16-7, reactions 2487-49-2, 7α-Hydroxyestrone 6803-21-0, 11β-Hydroxyestrone 10448-96-1, 7α-Methylestrone
RL: RCT (Reactant); RACT (Reactant or reagent)
(Wittig reaction of)
IT 1779-49-3, Methyltriphenylphosphonium bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(Wittig reaction of, with dehydroestrone)
IT 1530-32-1, Ethyltriphenylphosphonium bromide 1779-51-7, Butyltriphenylphosphonium bromide 6228-47-3, Propyltriphenylphosphonium bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(Wittig reaction of, with estrone)
IT 2208-12-0, 6-Dehydroestrone
RL: RCT (Reactant); RACT (Reactant or reagent)
(Wittig reaction of, with methyltriphenylphosphonium bromide)
IT 120661-79-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(chlorination of, with phosphorus oxytrichloride)
IT 50-28-2P, Estradiol, preparation
RL: PREP (Preparation)
(estrogenic and antifertility activity of)
IT 57-63-6 3762-05-8 34816-55-2 50866-95-0 59903-16-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(estrogenic and antifertility activity of)
IT 67530-18-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(fluorination of, with piperidinylsulfur trifluoride)
IT 120476-13-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrogenation of)
IT 100-53-8, Benzyl mercaptan
RL: RCT (Reactant); RACT (Reactant or reagent)
(ketalization by, of estrone)
IT 901-93-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(ketalization of, with benzyl mercaptan)
IT 917-54-4, Methyllithium
RL: RCT (Reactant); RACT (Reactant or reagent)
(methylation by, of hydroxynorpregnatrienone)
IT 591-51-5, Phenyllithium
RL: RCT (Reactant); RACT (Reactant or reagent)
(phenylation by, of estratetraenone derivative)
IT 17748-68-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(phenylation of, with phenyllithium)
IT 1787-44-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Wittig reaction of, with estrone)
IT 120476-12-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deacetylation of)
IT 120496-23-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and dehydrochlorination of)
IT 120475-89-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dehydroiodination of)
IT 117864-98-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deketalization of)
IT 120476-02-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and desilylation-dehydration of)
IT 3342-64-1P 5982-51-4P 7628-02-6P 16934-51-3P 59077-04-2P, 19-Norpregna-1,3,5(10)-trien-3-ol 59452-14-1P 59452-15-2P 59452-16-3P, 19,21-Dinorchola-1,3,5(10)-trien-3-ol 60037-62-9P 65928-98-5P 73271-91-7P 84510-05-4P 97560-70-8P, 19-Norpregna-1,3,5(10),20-tetraen-3-ol 108887-34-9P 120475-91-4P 120475-92-5P 120475-94-7P 120475-96-9P 120476-01-9P 120476-03-1P 120476-04-2P 120476-05-3P 120476-06-4P 120476-07-5P 120476-09-7P 120476-11-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and estrogenic and antifertility activity of)
IT 33946-34-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and fluorination by, of acetoxynorpregnatrienone)
IT 120475-95-8P 120476-08-6P 120476-10-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenation of)
IT 120475-88-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and iodination of)
IT 120475-99-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and selective de-O-methylation of)
IT 65929-00-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 4736-62-3P **34111-53-0P** 99898-92-7P, 19-Norpregna-1,3,5(10)-trien-20-yn-3-ol 102177-29-7P 120475-90-3P 120475-93-6P 120475-97-0P 120574-27-8P 120574-28-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, hydrogenation, and estrogenic and antifertility activity of)
IT 120475-98-1P 120476-00-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, methylation, and estrogenic and antifertility activity of)
IT 95943-73-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, reduction, and estrogenic and antifertility activity of)
IT 62437-99-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with estrone)
IT 994-30-9, Triethylchlorosilane
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ethynylestratriene derivative)
IT 7783-60-0, Sulfur tetrafluoride
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with piperidine derivative)
IT 3768-56-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with sulfur tetrafluoride)
IT 603-35-0, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with trideuteromethyl bromide)
IT 1111-88-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with triphenylphosphine)
IT 1667-98-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with hydrazine and estrogenic and antifertility activity of)
IT 120574-29-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(saponification of)
IT **34111-53-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, hydrogenation, and estrogenic and antifertility activity of)
RN 34111-53-0 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methylene- (7CI, 8CI, 9CI) (CA INDEX NAME)

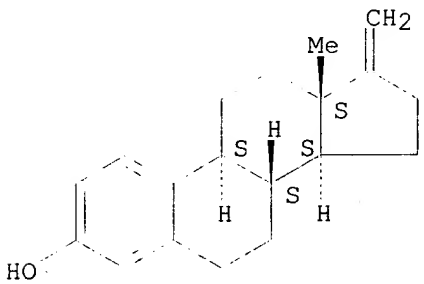
Absolute stereochemistry.



L89 ANSWER 17 OF 22 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 1981:462492 HCAPLUS
DN 95:62492
ED Entered STN: 12 May 1984
TI D-Homo steroids from oxidation of 17-methylene steroids by thallium(III) nitrate
AU Forcellese, Maria Luigia; Camerini, Elio; Ruffini, Bruna; Mincione, Enrico
CS Cent. Stud. Chim. Sostanze Org. Nat., CNR, Italy
SO Journal of Organic Chemistry (**1981**), 46(16), 3326-8
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
CC 32-4 (Steroids)
AB Thallium (III)-nitrate reacts with 17-methylene steroids to form D-homo-17α-methoxy-17a-oxo compds. via ring enlargement, enolization, oxythallation, and methanolysis.
ST methylene steroid thallium oxidn; homosteroid methoxyoxo
IT Rearrangement
(in thallium nitrate oxidation of methylene steroids, methoxyoxo homosteroids from)
IT Oxidation
(of methylene steroids by thallium nitrate, methoxyoxo homosteroids from)
IT D-Homosteroids
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, by thallium nitrate oxidation of methylene steroids)
IT 53-16-7P, preparation
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(methylenation of)
IT 13746-98-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation reagent, for methylene steroids)
IT **34111-53-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acetylation of)
IT 77257-05-7P 77257-07-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
IT 77257-04-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and hyrolysis of)
IT 77257-08-0P 77257-09-1P 77257-10-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 853-22-5 1164-94-9 77257-06-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(thallium nitrate oxidation of)
IT **34111-53-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acetylation of)
RN 34111-53-0 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methylene- (7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



L89 ANSWER 18 OF 22 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 1979:121859 HCAPLUS
DN 90:121859
ED Entered STN: 12 May 1984
TI Clinical analysis on steroids. Part V. Synthesis of 2,3,17β-trihydroxyestra-1,3,5(10)-trien-6-one and its related compounds
AU Nakagawa, Akiko; Ohuchi, Ryoko; Yoshizawa, Itsuo
CS Hokkaido Inst. Pharm. Sci., Hokkaido, Japan
SO Chemical & Pharmaceutical Bulletin (**1978**), 26(11), 3567-71
CODEN: CPBTAL; ISSN: 0009-2363
DT Journal
LA English
CC 32-3 (Steroids)
AB Allylic oxidation of 2,3-dimethoxy-17β-acetoxyestra-1,3,5(10)-triene and subsequent saponification gave 17β-hydroxy-2,3-dimethoxyestra-1,3,5(10)-trien-6-one, which was treated with pyridine containing HCl at 200° for 15 min to give 2,3,17β-trihydroxyestra-1,3,5(10)-trien-6-one.

Similarly, 3,17β-diacetoxy-2-methoxyestra-1,3,5(10)-triene gave 3,17β-dihydroxy-2-methoxyestra-1,3,5(10)-trien-6-one and 2,17β-diacetoxy-3-methoxyestra-1,3,5(10)-triene gave 2,17β-dihydroxy-3-methoxyestra-1,3,5(10)-triene-6-one.

ST oxidn allylic methoxyestratriene; estratrienol acetate allylic oxidn; estratrienone trihydroxy; methoxyestratrienone

IT Oxidation
(allylic, of unsatd. 19-norsteroids)

IT 19-Norsteroids
RL: RCT (Reactant); RACT (Reactant or reagent)
(unsatd., allylic oxidation of)

IT 5976-65-8 5976-67-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(acetylation of)

IT **7291-57-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(allylic oxidation of)

IT 69540-61-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acetylation of)

IT 5976-70-5P 7002-81-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and allylic oxidation of)

IT 69540-59-6P 69540-62-1P 69591-42-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deacetylation of)

IT 69540-60-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and demethylation of)

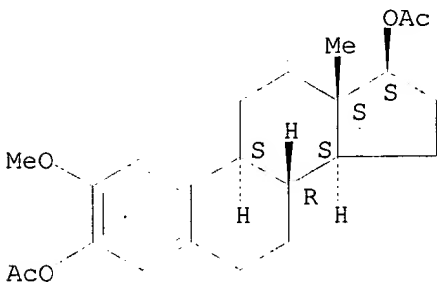
IT 68129-02-2P 69540-63-2P 69540-64-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT **7291-57-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(allylic oxidation of)

RN 7291-57-8 HCAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-, diacetate, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L89 ANSWER 19 OF 22 HCAPLUS COPYRIGHT 2003 ACS on STN

AN 1976:421725 HCAPLUS

DN 85:21725

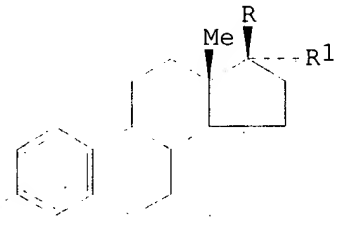
ED Entered STN: 12 May 1984

TI 19-Norpregna-1,3,5(10)-trien-3-ol and lower alkyl homologs having

postcoital antifertility activity
IN Crowe, David F.; Peters, Richard H.; Tanabe, Masato; Detre, George
PA Stanford Research Institute, USA
SO U.S., 5 pp.
CODEN: USXXAM
DT Patent
LA English
IC C07J
NCL 260397500
CC 32-5 (Steroids)
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 3946052	A	19760323	US 1975-587256	19750616 <--
PRAI US 1975-587256		19750616 <--		

GI



I

AB Estratrienols I (R = Me, Et, Pr, Bu; R1 = H) were prepared by Wittig reaction of I (RR1 = O) with RP+Ph3 Br- followed by hydrogenation over Pd/C. Thus, a solution of 9.5 g estrone in Me2SO was added to a suspension of EtP+Ph3 Br- and NaH in Me2SO. Heating the mixture for 18 hr at 60° yielded 6.8 g I (RR1 = CHMe). Hydrogenation of 500 mg I (RR1 = CHMe) over Pd/C gave 400 mg I (R = Et, R1 = H), which had a 100 fold separation of postcoital antifertility from estrogenic activity as compared with ethynylestradiol at 200μg/hk/day orally in rats.

ST norpregnatrienol contraceptive; Wittig estrone; norpregnatetraene hydrogenation

IT 19-Norsteroids
RL: RCT (Reactant); RACT (Reactant or reagent)
(17β-alkyl-3-hydroxy-1,3,5(10)-unsatd.)

IT Contraceptives
(postcoital, 19-norpregna-1,3,5(10)-trien-3-ol as)

IT 53-16-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(Wittig reaction of)

IT 4350-65-6P **34111-53-0P** 59452-12-9P 59452-13-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenation of)

IT 59077-04-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and postcoital antifertility activity of)

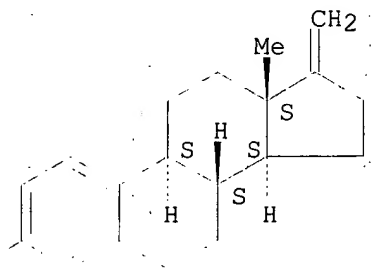
IT 59452-14-1P 59452-15-2P 59452-16-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 1530-32-1 1779-49-3 1779-51-7 6228-47-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with estrone)

IT **34111-53-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrogenation of)
RN 34111-53-0 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methylene- (7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

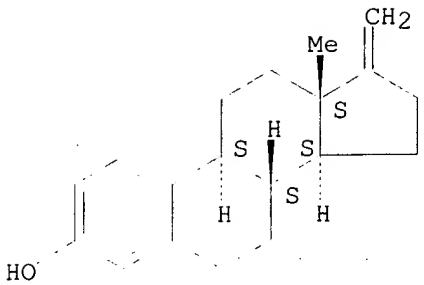


L89 ANSWER 20 OF 22 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 1971:551978 HCAPLUS
DN 75:151978
ED Entered STN: 12 May 1984
TI 17-Methyleneestrane derivatives
IN Ota, Motokichi; Takegoshi, Toshio; Obata, Kazunaga; Oshima, Yasuo; Kasahara, Akira
PA Daiichi Seiyaku Co., Ltd.
SO Jpn. Tokkyo Koho, 4 pp.
CODEN: JAXXAD
DT Patent
LA Japanese
IC C07C; C07D; A61K
CC 32 (Steroids)
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 46034421	B4	19711008	JP	19681208 <--

AB 17-Oxoestrane derivative was treated with (Ph3PMe)X (X=halogen) in the presence of an acidic condensation agent to give the corresponding 17-methyleneestrane derivative Thus, estrone and (Ph3PMe)Br in Me2SO was stirred with tert-BuOK in a N stream to give 17-methyleneestra-1,3,5(10)-trien-3-ol. Similarly prepared were 3 more 3-substituted 17-methyleneestra-1,3,5(10)-trienes. The products are anticholesterol agents.
ST estrane methylene derivs; anticholesterol estranes
IT **34111-53-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **34111-53-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 34111-53-0 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methylene- (7CI, 8CI, 9CI) (CA INDEX NAME)

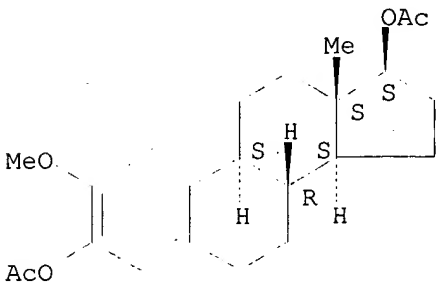
Absolute stereochemistry.



L89 ANSWER 21 OF 22 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 1970:516788 HCAPLUS
DN 73:116788
ED Entered STN: 12 May 1984
TI Analytical chemical studies on steroids. XXXVII. Gas chromatography of 2,3-oxygenated estratrienes
AU Nambara, Toshio; Iwata, Takehiko; Honma, Seijiro
CS Pharm. Inst., Tohoku Univ., Sendai, Japan
SO Journal of Chromatography (**1970**), 50(3), 400-4
CODEN: JOCRAM; ISSN: 0021-9673
DT Journal
LA English
CC 4 (Hormones and Related Substances)
AB The steroid number (SN) values (W. Van de Heuvel and E. C. Horning, 1962) for estratrienes having O functional group substituents at the 2- and 3-positions were determined by gas chromatog. on a 3% SE-3/Chromosorb W column, with a H flame ionization detector and N carrier gas. The SN contributions of various O functional groups at the 2- and 3-positions were estimated by using estra-1,3,5(10)-triene as a reference compound The contribution of 2 functional groups on ring A and D was in agreement with the summation of the values characteristic of each substituent. The additivity rule was applicable to the 2,3-oxygenated estratrienes, when the SN contributions of the vicinal functional groups on ring A are considered as a set. The method may be used to identify metabolites derived from modified steroids as well as the naturally occurring estrogens.
ST steroids gas chromatog; estratrienes gas chromatog; gas chromatog estratrienes
IT Steroids, properties
RL: PROC (Process)
(chromatog. of)
IT Molecular structure-property relationships
(chromatographic, of estratriene derivs.)
IT 50-28-2, analysis 53-16-7, analysis 53-45-2 53-63-4 362-07-2
362-08-3 901-93-9 1035-77-4 1217-09-0 1549-15-1 1743-60-8
1839-54-9 2259-89-4 2354-44-1 2529-64-8 2755-14-8 3434-88-6
4967-94-6 5150-62-9 5976-55-6 5976-59-0 5976-63-6 5976-65-8
7002-81-5 **7291-57-8** 10584-10-8 10584-11-9 14550-57-3
16274-22-9 17519-71-0 17553-16-1 18880-67-6 26356-97-8
26356-99-0 29741-91-1 29741-92-2 29741-94-4 29755-23-5
29755-24-6 29755-25-7 29755-26-8 29755-30-4 29755-31-5
29755-32-6 29755-33-7 29755-34-8 29755-43-9 29825-35-2
29825-36-3 29825-37-4 29825-39-6 29825-40-9 29825-41-0
29825-42-1 29825-43-2 29825-44-3 29825-46-5 29825-47-6
29825-48-7 29971-45-7 29971-46-8 29978-30-1
RL: PROC (Process)
(chromatog. of)
IT **7291-57-8**
RL: PROC (Process)

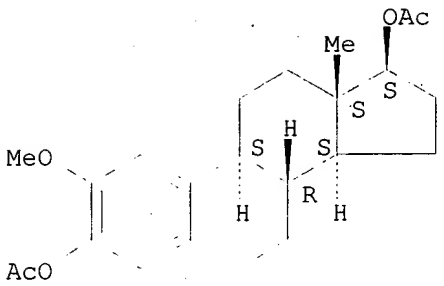
(chromatog. of)
RN 7291-57-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-, diacetate, (17β)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



L89 ANSWER 22 OF 22 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 1970:121765 HCAPLUS
DN 72:121765
ED Entered STN: 12 May 1984
TI Analytical chemical studies on steroids. XXXIII. Steroid conjugates. III. New syntheses of 2-methoxyestrogens
AU Nambara, Toshio; Honma, Seijiro; Akiyama, Setsuko
CS Pharm. Inst., Tohoku Univ., Sendai, Japan
SO Chemical & Pharmaceutical Bulletin (**1970**), 18(3), 474-80
CODEN: CPBTAL; ISSN: 0009-2363
DT Journal
LA English
CC 32 (Steroids)
OS CASREACT 72:121765
AB New synthetic routes leading to the 2-methoxyestrogens from the readily av ailable compds. were investigated. Utilization of both Friedel-Crafts and Baeyer-Villiger reactions wit h estrone and estradiol 3-methyl ethers gave the desired 2-methoxyestrogen s in overall yield of .apprx.50%. Fries rearrangement with estrone acetate and Friedel-Crafts reaction with 2-methoxy-3-deoxyestrogens were also undertaken. The chemical shifts of the aromatic protons of the 2,3-substituted estratrienes are collected in tables.
ST estrogens methoxy; methoxy estrogens; estrenols methoxy
IT 19-Norsteroids
RL: RCT (Reactant); RACT (Reactant or reagent)
(2-methoxy)
IT 362-07-2P 362-08-3P 2259-89-4P **7291-57-8P** 17519-71-0P
17553-16-1P 26356-51-4P 26356-52-5P 26356-53-6P 26356-54-7P
26356-93-4P 26356-96-7P 26356-97-8P 26356-99-0P 26357-00-6P
26357-02-8P 26357-03-9P 26357-04-0P 26357-05-1P 26357-06-2P
26357-07-3P 26362-43-6P 26362-44-7P 26517-50-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **7291-57-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 7291-57-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-, diacetate, (17β)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



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L80 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 2003:719252 HCAPLUS
DN 139:224972
ED Entered STN: 14 Sep 2003
TI Synthesis of 2-methoxyestradiol derivatives and uses as antiangiogenic agents
IN **Lavallee, Theresa M.; Pribluda, Victor S.**; Simons, Jonathan; Mabjeesh, Nicola; Giannakakou, Paraskevi
PA **Entremed, Inc., USA**
SO PCT Int. Appl., 77 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM A61K
CC 2-4 (Mammalian Hormones)
Section cross-reference(s): 32
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003073985	A2	20030912	WO 2003-US5898	20030227 <--

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2002-361267P P 20020301 <--
AB Compns. and methods for treating mammalian disease characterized by undesirable angiogenesis and for controlling a number of angiogenesis-related events, conditions, or substances, by administering derivs. of 2-methoxyestradiol of general formula (I) wherein the variables are defined in the specification.
ST estrogen methoxyestradiol analogs angiogenesis inhibitor VEGF DR5 HIFalpha
IT Apoptosis
(2-ME2-induced; synthesis of 2-methoxyestradiol derivs. and uses as antiangiogenic agents)
IT Cytokine receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(DR5 (death receptor 5); synthesis of 2-methoxyestradiol derivs. and uses as antiangiogenic agents)
IT Transcription factors

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(HIF-1α (hypoxia-inducible factor 1α); synthesis of
2-methoxyestradiol derivs. and uses as antiangiogenic agents)

IT Blood vessel
(endothelium; synthesis of 2-methoxyestradiol derivs. and uses as
antiangiogenic agents)

IT Transcriptional regulation
(of HIF-1α, 2-ME2-inhibited; synthesis of 2-methoxyestradiol
derivs. and uses as antiangiogenic agents)

IT Angiogenesis
Angiogenesis inhibitors
Human
(synthesis of 2-methoxyestradiol derivs. and uses as antiangiogenic
agents)

IT Estrogens
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
(Biological study); PREP (Preparation)
(synthesis of 2-methoxyestradiol derivs. and uses as antiangiogenic
agents)

IT 127464-60-2, Vascular Endothelial Growth Factor
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(synthesis of 2-methoxyestradiol derivs. and uses as antiangiogenic
agents)

IT 362-07-2DP, 2-Methoxyestradiol, derivs. and analogs 362-07-2P,
2-Methoxyestradiol
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant
or reagent)
(synthesis of 2-methoxyestradiol derivs. and uses as antiangiogenic
agents)

IT 50-00-0, Formaldehyde, reactions 50-28-2D, Estradiol, derivs. and
analogs 53-16-7, Estrone, reactions 64-18-6, Formic acid, reactions
64-19-7, Acetic acid, reactions 67-68-5, Methyl sulfoxide, reactions
68-12-2, DMF, reactions 71-36-3, 1-Butanol, reactions 75-09-2,
Methylene chloride, reactions 79-37-8, Oxalyl chloride 100-39-0,
Benzyl bromide 106-95-6, Allyl bromide, reactions 109-99-9, THF,
reactions 111-46-6, Diethylene glycol, reactions 121-44-8,
Triethylamine, reactions 141-78-6, Ethyl acetate, reactions 302-01-2,
Hydrazine, reactions 362-08-3, 2-Methoxyestrone 362-08-3D,
2-Methoxyestrone, olefin analogs 584-08-7, Potassium carbonate
1157-87-5, AH3 1530-32-1, Ethyl triphenylphosphonium bromide
1779-49-3, Methyltriphenylphosphonium bromide 1779-51-7, Butyl
triphenylphosphonium bromide 4111-54-0, Lithium diisopropyl amide
4784-77-4, Crotyl bromide 5815-08-7, tert-Butoxy
bis(dimethylamino)methane 6228-47-3, Propyl triphenylphosphonium bromide
7447-41-8, Lithium chloride, reactions 7632-00-0, Sodium nitrite
7693-26-7, Potassium hydride 16853-85-3, Lithium aluminum hydride
17455-13-9, 18-Crown-6 17640-15-2, Methyl cyanoformate 41233-93-6,
Potassium-tert-amylate 431901-79-0 431901-81-4 431901-84-7
431901-85-8 431901-89-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of 2-methoxyestradiol derivs. and uses as antiangiogenic
agents)

IT 53-63-4P, Estra-1,3,5(10)-trien-3-ol
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(synthesis of 2-methoxyestradiol derivs. and uses as antiangiogenic
agents)

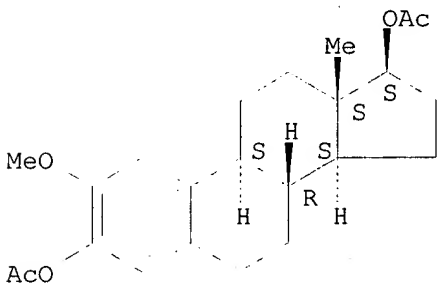
IT 362-07-2DP, 2-Methoxyestradiol, alkyl analogs 4953-96-2P 6298-51-7P
6301-87-7P 6599-97-9P **7291-57-8P** 10332-20-4P 26356-54-7DP,
alkyl derivs 26356-54-7DP, alkyl derivs. 26356-54-7P 26357-07-3DP,
16α-alkyl derivs. 26357-07-3P 32162-96-2P **34111-53-0P**
93949-26-9P 165619-07-8P **229486-18-4P 431901-68-7P**

431901-69-8P **431901-70-1P 431901-71-2P** 431901-72-3P
431901-77-8P 431901-78-9P 431901-80-3DP, alkyl derivs.
431901-89-2DP, alkyl analogs 431901-90-5P 431901-91-6P 431901-92-7P
431901-93-8P 431901-98-3P 431901-99-4P 431902-01-1P 431902-02-2P
431902-03-3P 431902-04-4P 431902-05-5P 431902-06-6P 431902-09-9P
438044-30-5P 464924-32-1P 594873-85-5P 594873-86-6P 594873-87-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of 2-methoxyestradiol derivs. and uses as antiangiogenic agents)

IT **7291-57-8P 34111-53-0P 229486-18-4P**
431901-68-7P 431901-70-1P 431901-71-2P
431901-77-8P 431901-78-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of 2-methoxyestradiol derivs. and uses as antiangiogenic agents)

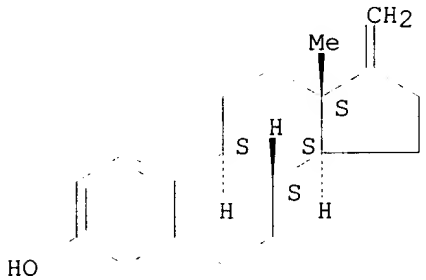
RN 7291-57-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-, diacetate, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



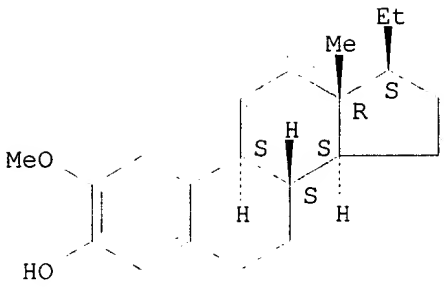
RN 34111-53-0 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methylene- (7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



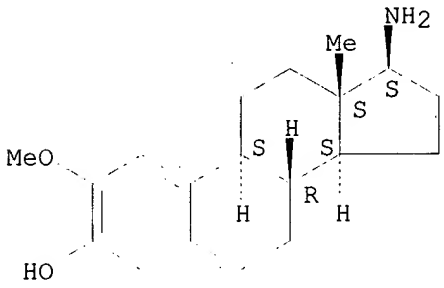
RN 229486-18-4 HCAPLUS
CN 19-Norpregna-1,3,5(10)-trien-3-ol, 2-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



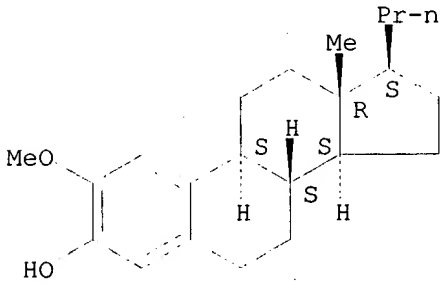
RN 431901-68-7 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-amino-2-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



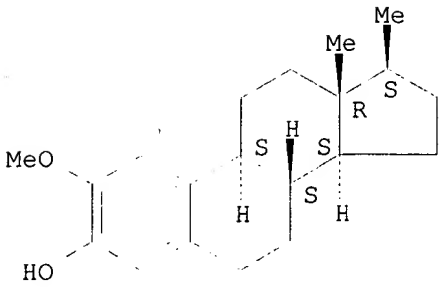
RN 431901-70-1 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 2-methoxy-17-propyl-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



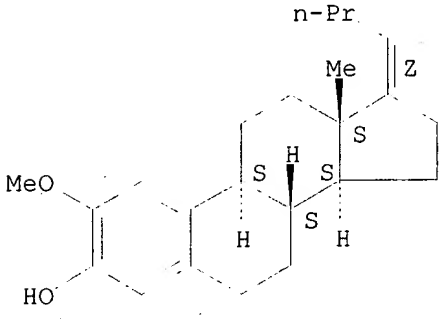
RN 431901-71-2 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 2-methoxy-17-methyl-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



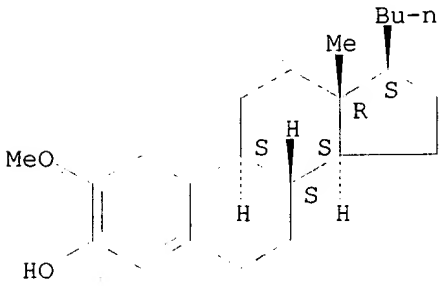
RN 431901-77-8 HCAPLUS
CN 19,21-Dinorchola-1,3,5(10),17(20)-tetraen-3-ol, 2-methoxy-, (17Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 431901-78-9 HCAPLUS
CN 19,21-Dinorchola-1,3,5(10)-trien-3-ol, 2-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

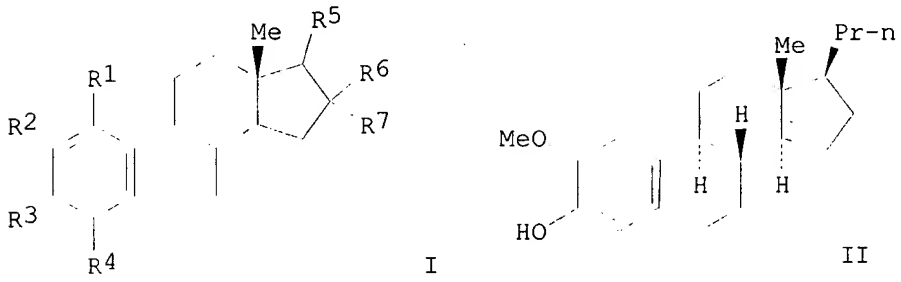


L80 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 2002:488275 HCAPLUS
DN 137:47357
ED Entered STN: 28 Jun 2002
TI Preparation of 2-methoxyestradiol derivatives as antiangiogenic agents
IN **Agoston, Gregory E.; Shah, Jamshed H.; Hunsucker, Kimberly A.; Pribluda, Victor S.; Lavallee, Theresa M.; Green, Shawn J.; Herbstritt, Christopher J.; Zhan, Xiaoguo H.; Treston, Anthony M.**
PA USA
SO U.S. Pat. Appl. Publ., 37 pp., Cont.-in-part of U. S. Ser. No. 933,894.
CODEN: USXXCO

DT Patent
LA English
IC ICM C07J041-00
ICS C07J043-00; C07J001-00; A61K031-704; A61K031-58; A61K031-56; C07C247-00; A61K031-655; C07J009-00
NCL 552544000
CC 32-3 (Steroids)
Section cross-reference(s): 1
FAN.CNT 2

	PATENT NO.	KIND	DATE		APPLICATION NO.	DATE
PI	US 2002082433	A1	20020627		US 2001-939208	20010824 <--
PRAI	US 2000-641327	A2	20000818	<--		
	US 2000-253385P	P	20001127	<--		
	US 2000-255302P	P	20001213	<--		
	US 2001-278250P	P	20010323	<--		
	US 2001-933894	A2	20010821	<--		

OS MARPAT 137:47357
GI



AB 2-Methoxyestradiol derivs. of formula I [R1, R4 = H, halo, CN, alkyl, OH, NH2, etc.; R2 = N3, CN, OMe, alkenyl, alkynyl, alkoxy, NH2, etc.; R3 = OH, OAc; R5 = alkyl, alkenyl, (di)alkylamino, OH, alkylene, etc.; R6, R7 = H, alkyl, alkenyl, alkynyl, halo, etc.] are prepared for treating mammalian disease characterized by undesirable angiogenesis. Thus, II was prepared from 2-methoxyestradiol and propyltriphenylphosphonium bromide. The IC50 of II against MDA-MB-231 breast tumor cells was 51.31 μM.

ST methoxyestradiol deriv prepn antiangiogenic; estradiol deriv prepn antiangiogenic; antitumor methoxyestradiol deriv prepn; antimitotic methoxyestradiol deriv prepn

IT Structure-activity relationship
(antitumor; preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT Mitosis
(inhibitors; preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT Angiogenesis inhibitors
Antitumor agents
Human
Mammary gland, neoplasm
Neoplasm
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT 362-07-2, 2-Methoxyestradiol
RL: PAC (Pharmacological activity); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT 53-63-4P, Estra-1,3,5(10)-trien-3-ol 6301-87-7P 431901-72-3P 431901-73-4P 431901-75-6P **431901-77-8P** 431901-91-6P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic

preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT 1818-12-8P 4953-96-2P 6298-51-7P 6599-97-9P **7291-57-8P**
10332-20-4P 32162-96-2P 41259-43-2P 94440-60-5P 165619-07-8P
165881-61-8P **229486-18-4P 431901-68-7P** 431901-69-8P
431901-70-1P 431901-71-2P 431901-74-5P
431901-78-9P 431901-87-0P 431901-90-5P 431901-92-7P
431901-93-8P 431901-94-9P 431901-95-0P 431901-96-1P
431901-97-2P 431901-98-3P 431901-99-4P 431902-00-0P
431902-01-1P 431902-02-2P 431902-03-3P 431902-04-4P 431902-05-5P
431902-06-6P 431902-07-7P 431902-08-8P 431902-09-9P
438044-29-2P 438044-30-5P 438044-35-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

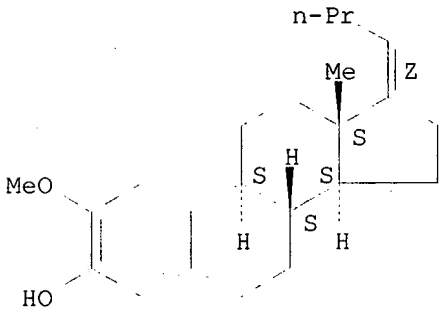
IT 53-16-7, Estrone, reactions 106-95-6, Allyl bromide, reactions
1779-51-7, Butyltriphenylphosphonium bromide 4784-77-4, Crotyl bromide
5815-08-7 6228-47-3, Propyltriphenylphosphonium bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT 26356-54-7P 26357-07-3P 93949-26-9P 431901-79-0P 431901-81-4P
431901-82-5P 431901-83-6P 431901-84-7P 431901-85-8P 431901-89-2P
438044-31-6P 438044-32-7P 438044-33-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT **431901-77-8P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

RN 431901-77-8 HCAPLUS
CN 19,21-Dinorchola-1,3,5(10),17(20)-tetraen-3-ol, 2-methoxy-, (17Z)- (9CI) (CA INDEX NAME)

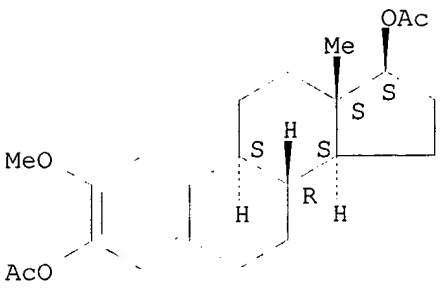
Absolute stereochemistry.
Double bond geometry as shown.



IT **7291-57-8P 229486-18-4P 431901-68-7P**
431901-70-1P 431901-71-2P 431901-74-5P
431901-78-9P 431901-97-2P 438044-29-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

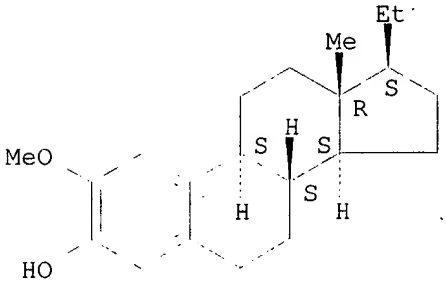
RN 7291-57-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-, diacetate, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



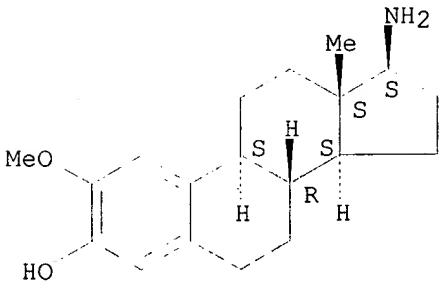
RN 229486-18-4 HCAPLUS
CN 19-Norpregna-1,3,5(10)-trien-3-ol, 2-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



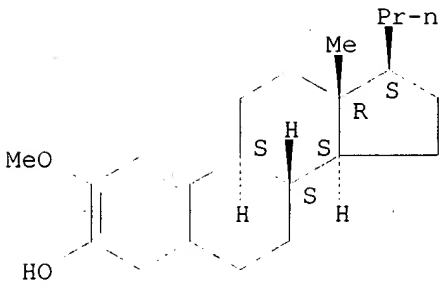
RN 431901-68-7 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-amino-2-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



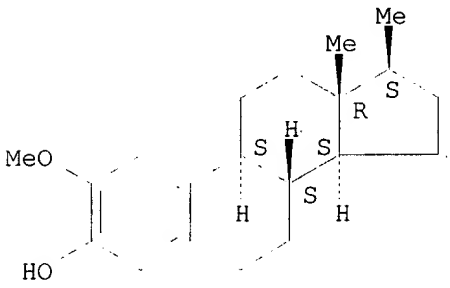
RN 431901-70-1 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 2-methoxy-17-propyl-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



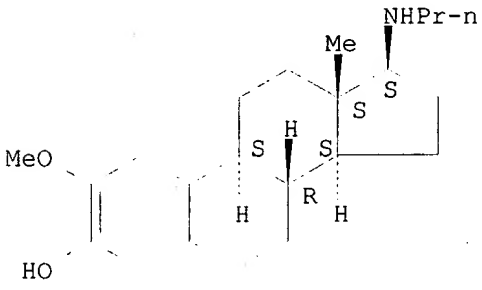
RN 431901-71-2 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 2-methoxy-17-methyl-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



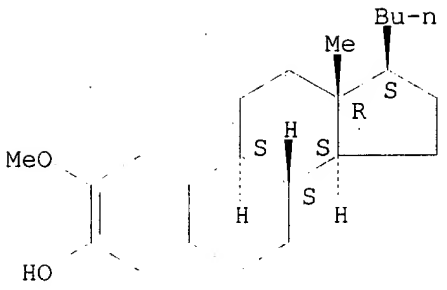
RN 431901-74-5 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 2-methoxy-17-(propylamino)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



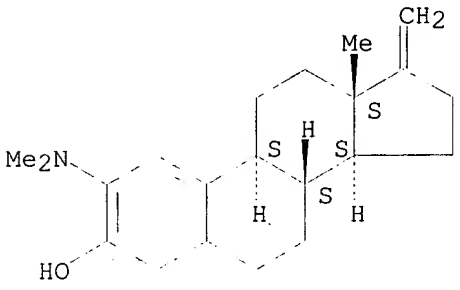
RN 431901-78-9 HCAPLUS
CN 19,21-Dinorchola-1,3,5(10)-trien-3-ol, 2-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 431901-97-2 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 2-(dimethylamino)-17-methylene-, hydrochloride (9CI) (CA INDEX NAME)

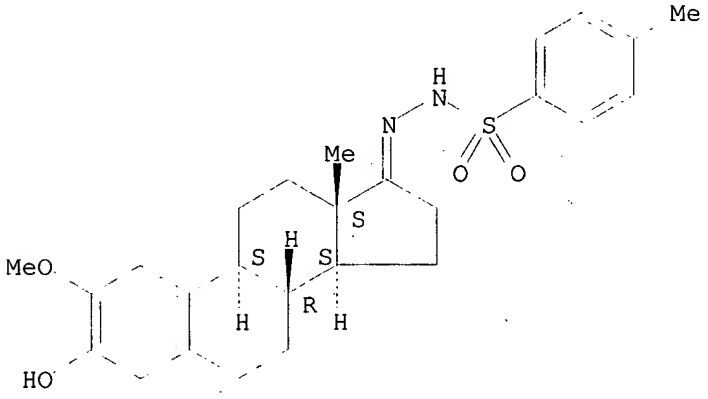
Absolute stereochemistry.



● HCl

RN 438044-29-2 HCAPLUS
CN Benzenesulfonic acid, 4-methyl-, (3-hydroxy-2-methoxyestra-1,3,5(10)-trien-17-ylidene)hydrazide (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



L80 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 2002:408687 HCAPLUS
DN 137:6309
ED Entered STN: 31 May 2002

TI Preparation of 2-methoxyestradiol analogs as antiangiogenic agents

IN **Agoston, Gregory; Shah, Jamshed H.; Hunsucker, Kimberly A.; Pribluda, Victor; Lavallee, Theresa M. ; Green, Shawn J.; Herbstritt, Christopher J.; Zhan, Xiaoguo H.; Treston, Anthony**

PA **Entremed, Inc., USA**

SO PCT Int. Appl., 86 pp.
CODEN: PIXXD2

DT Patent

LA English

IC ICM C07J001-00

CC 32-3 (Steroids)
Section cross-reference(s): 1, 2, 63

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	WO 2002042319	A2	20020530	WO 2001-US26490	20010824	<--
	WO 2002042319	A3	20030313			
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	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
	AU 2001088386	A5	20020603	AU 2001-88386	20010824	<--
	EP 1343803	A2	20030917	EP 2001-968112	20010824	<--
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PRAI	US 2000-253385P	P	20001127 <--
	US 2000-255302P	P	20001213 <--
	US 2001-278250P	P	20010323 <--
	US 2001-933894	A	20010821 <--
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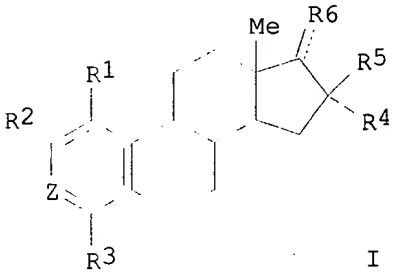
OS MARPAT 137:6309

GI



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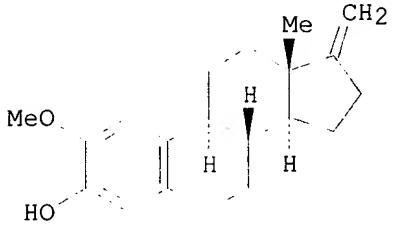


II

AB 2-Methoxyestradiol analogs, such as I [R1, R3 = H, halo, CN, alkyl, OH, CH2OH, NH2, alkylamino; R2 = N3, CN, C.tplbond.CR, C=CHR, C.tplbond.CH, OR, amino; R = H, alkyl; Z = COH, COAc; dashed bond = single bond or double bond; R6 = H, OH, O, oxime, amino, alkyl, alkenyl; R4, R5 = H, alkyl, alkenyl, alkynyl], were prepared for treating mammalian disease characterized by undesirable angiogenesis. Thus, 2-methoxyestradiol analog II was prepared by the reaction of methyltriphenylphosphonium bromide and 2-methoxyestrone. In vitro evaluation against MDA-MB-231 breast tumor cells and HUVEC endothelial cells, II showed IC50 0.24±0 and 0.19±0.19 resp.

ST methoxyestradiol deriv prepn antiangiogenic antitumor; estradiol methoxy deriv prepn antiangiogenic antitumor

IT Cell proliferation
(inhibition; preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT Mammary gland, neoplasm
(inhibitors; preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT Antitumor agents
(mammary gland; preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT Angiogenesis inhibitors
Human
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT Estrogens
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT 53-63-4P, Estra-1,3,5(10)-trien-3-ol 431901-72-3P 431901-73-4P
431901-75-6P **431901-77-8P** 431901-83-6P 431901-89-2P
431901-91-6P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT 1818-12-8P 4953-96-2P 6298-51-7P 6301-87-7P 6599-97-9P
7291-57-8P 10332-20-4P 32162-96-2P 41259-43-2P 94440-60-5P
165619-07-8P 165881-61-8P 192062-02-5P **229486-18-4P**
431901-68-7P 431901-69-8P **431901-70-1P**
431901-71-2P **431901-74-5P** **431901-76-7P**
431901-78-9P 431901-82-5P 431901-84-7P 431901-86-9P
431901-87-0P 431901-88-1P 431901-92-7P 431901-93-8P 431901-94-9P
431901-95-0P 431901-96-1P **431901-97-2P** 431901-98-3P
431901-99-4P 431902-00-0P 431902-01-1P 431902-02-2P 431902-03-3P
431902-04-4P 431902-05-5P 431902-06-6P 431902-07-7P 431902-08-8P
431902-09-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT 53-16-7, Estrone, reactions 64-18-6, Formic acid, reactions 100-39-0, Benzyl bromide 106-95-6, Allyl bromide, reactions 362-07-2, 2-Methoxyestradiol 1530-32-1, Ethyl triphenylphosphonium bromide 1779-49-3, Methyl triphenylphosphonium bromide 1779-51-7, Butyl triphenylphosphonium bromide 4784-77-4, Crotyl bromide 5815-08-7, tert-Butoxy bis(dimethylamino)methane 6228-47-3, Propyl triphenylphosphonium bromide 17640-15-2, Methyl cyanoformate
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

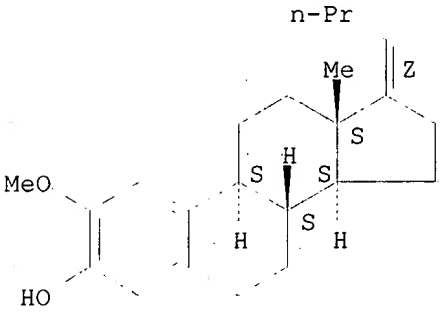
IT 26356-54-7P 26357-07-3P 93949-26-9P 431901-79-0P 431901-80-3P
431901-81-4P 431901-85-8P 431901-90-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

IT **431901-77-8P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

RN 431901-77-8 HCAPLUS

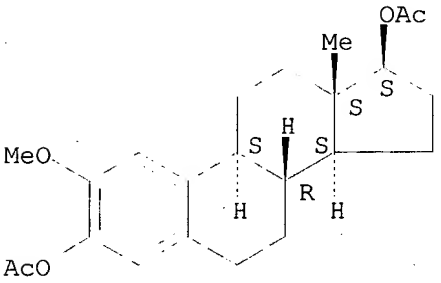
CN 19,21-Dinorchola-1,3,5(10),17(20)-tetraen-3-ol, 2-methoxy-, (17Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



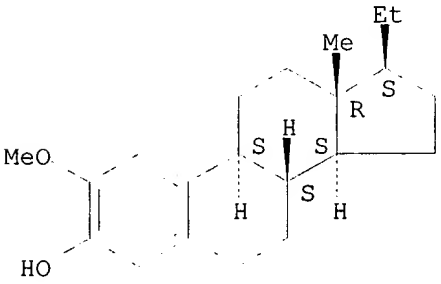
IT **7291-57-8P 229486-18-4P 431901-68-7P**
431901-70-1P 431901-71-2P 431901-74-5P
431901-76-7P 431901-78-9P 431901-97-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)
RN 7291-57-8 HCAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-, diacetate, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



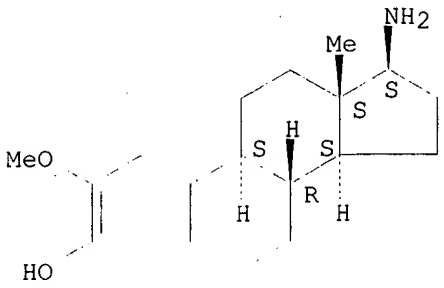
RN 229486-18-4 HCAPLUS
CN 19-Norpregna-1,3,5(10)-trien-3-ol, 2-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



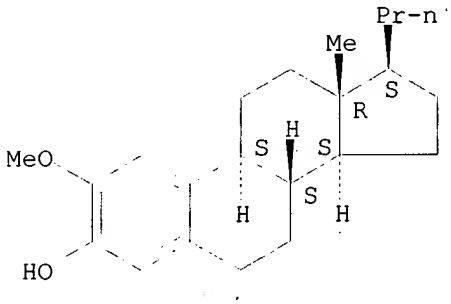
RN 431901-68-7 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-amino-2-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



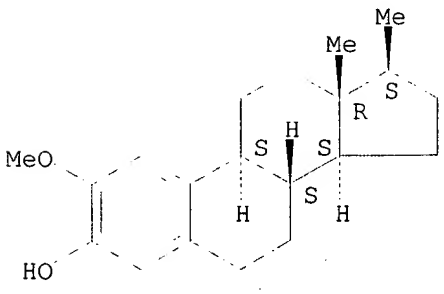
RN 431901-70-1 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 2-methoxy-17-propyl-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



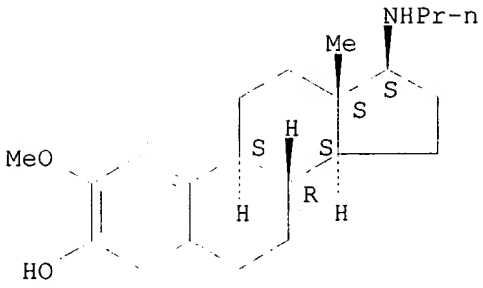
RN 431901-71-2 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 2-methoxy-17-methyl-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



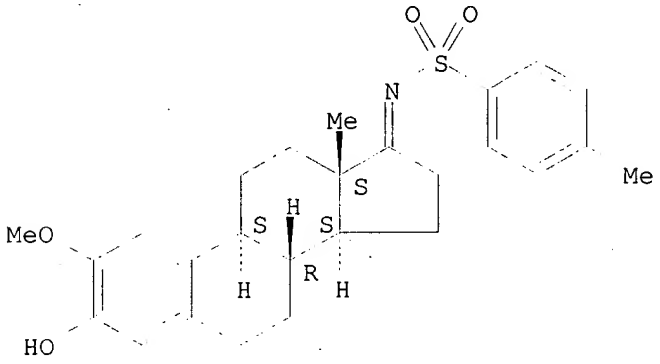
RN 431901-74-5 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 2-methoxy-17-(propylamino)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



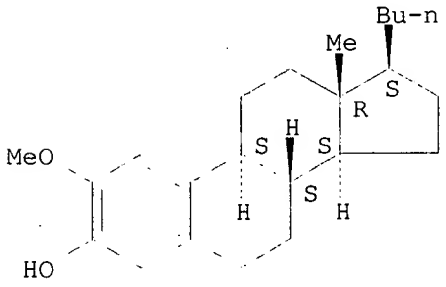
RN 431901-76-7 HCAPLUS
CN Benzenesulfonamide, N-(3-hydroxy-2-methoxyestra-1,3,5(10)-trien-17-ylidene)-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



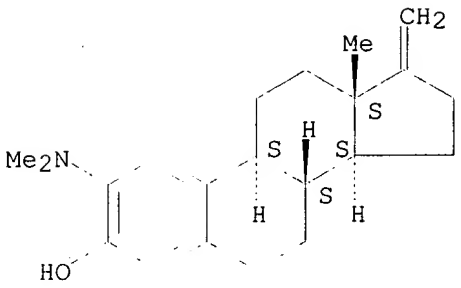
RN 431901-78-9 HCAPLUS
CN 19,21-Dinorchola-1,3,5(10)-trien-3-ol, 2-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 431901-97-2 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 2-(dimethylamino)-17-methylene-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

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=> d his

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               DEL HIS

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               SET COST OFF
L1          428 S E3 AND C5-C6-C6-C6/ES AND 4/NR
L2            8 S L1 AND 17 METHYLENE
L3            1 S L2 AND 2 METHOXY
               SEL RN
L4            0 S E1/CRN

     FILE 'HCAOLD' ENTERED AT 09:13:35 ON 21 DEC 2003
L5            0 S L3

     FILE 'USPATFULL, USPAT2' ENTERED AT 09:13:39 ON 21 DEC 2003
L6            1 S L3

     FILE 'HCAPLUS' ENTERED AT 09:13:41 ON 21 DEC 2003
L7            2 S L3

     FILE 'REGISTRY' ENTERED AT 09:14:10 ON 21 DEC 2003

     FILE 'USPATFULL, USPAT2' ENTERED AT 09:14:17 ON 21 DEC 2003

     FILE 'HCAPLUS' ENTERED AT 09:14:30 ON 21 DEC 2003

     FILE 'REGISTRY' ENTERED AT 09:15:35 ON 21 DEC 2003
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               E C5-C6-C6-C6/ES
L8       243537 S E3
L9             STR
L10           50 S L9 CSS SAM SUB=L8
L11         4643 S L9 CSS FUL SUB=L8
               SAV TEMP L11 QAZI939/A
L12            STR L9
L13            STR L9
L14           50 S L13 CSS SAM SUB=L8
L15         4643 S L13 CSS FUL SUB=L8
               SAV L15 QAZI939A/A
L16            3 S L12 CSS SAM SUB=L15
L17           50 S L12 CSS FUL SUB=L15
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                SAV L17 QAZI939B/A
L18          4593 S L15 NOT L17
L19               STR L12
                  DEL QAZI939/A
                  DEL QAZI939B/A
L20               STR L19
L21            50 S L20 CSS SAM SUB=L15
L22          1158 S L20 CSS FUL SUB=L15
                  SAV L22 QAZI939B/A
L23          3485 S L15 NOT L22
                  SAV L23 QAZI939C/A
L24               STR L20
L25             0 S L24 CSS SAM SUB=L15
L26            10 S L24 CSS FUL SUB=L15
                  SAV L26 QAZI939D/A
L27             9 S L26 NOT L3
L28               STR
L29             0 S L28 CSS SAM SUB=L15
L30               STR L28
L31             0 S L30 CSS SAM SUB=L15
L32             0 S L30 CSS FUL SUB=L15
                  SAV L32 QAZI939E/A
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L34             0 S L33 CSS SAM SUB=L15
L35             0 S L33 CSS FULL SUB=L15
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L36             0 S L27

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L37             5 S L27

     FILE 'HCAPLUS' ENTERED AT 09:46:41 ON 21 DEC 2003
L38             9 S L27
L39             2 S L38 AND ENTREMED?/PA,CS
L40             3 S L38 AND (AGOSTON ? OR SHAH ? OR HUNSUCKER ? OR PRIBLUDA ? OR
L41             9 S L38-L40

     FILE 'REGISTRY' ENTERED AT 09:48:58 ON 21 DEC 2003

     FILE 'USPATFULL, USPAT2' ENTERED AT 09:49:31 ON 21 DEC 2003

     FILE 'HCAPLUS' ENTERED AT 09:49:47 ON 21 DEC 2003
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L43             2 S (WO2001-US26490 OR US2001-933894# OR WO2001-US26128 OR US2001
L44             3 S L42,L43
L45             1 S L39,L40 NOT L44
L46             1 S US2002-361267#/AP,PRN
L47             4 S L44,L46
                  E AGOSTON G/AU
L48            24 S E5,E9,E10
                  E SHAH J/AU
L49           148 S E3,E9
                  E SHAH JAMSHED/AU
L50            29 S E3,E4,E5
                  E HUNSUCKER K/AU
L51             7 S E4,E5
                  E PRIBLUDA V/AU
L52            35 S E3-E8
                  E LAVALLEE T/AU
L53            16 S E4,E5
                  E LA VALLEE T/AU
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                E GREEN S/AU
L54          196 S E3,E15,E16
                E GREEN SHAWN/AU
L55           60 S E3-E5
                E HERBSTRITT C/AU
L56            7 S E4-E6
                E ZHAN X/AU
L57           31 S E3,E8
                E ZHAN XIA/AU
L58            6 S E38,E39
                E TRESTON A/AU
L59           54 S E3-E8
                E ENTREMED/PA,CS
L60           79 S E3-E15

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L61         4633 S L15 NOT L3,L26

     FILE 'HCAPLUS' ENTERED AT 09:59:04 ON 21 DEC 2003
L62        63865 S L61
L63            4 S L62 AND L47
L64           18 S L62 AND L48-L60
L65           14 S L64 NOT L63
                SEL HIT RN L63
                SEL HIT RN L65

     FILE 'REGISTRY' ENTERED AT 10:00:20 ON 21 DEC 2003
L66           54 S E1-E54
L67           11 S E55-E65
L68           50 S L66 NOT L67
L69           11 S L68 AND (C23H32O2 OR C23H24O2 OR C22H33NO2 OR C19H27NO2 OR C2
L70            9 S L69 NOT C20H28O2
L71            2 S L69 NOT L70
L72            1 S L71 NOT 165881-61-8
L73           10 S L70,L72
L74           40 S L68 NOT L73
L75            2 S L74 AND (C23H34O2 OR C26H32N2O4S)
L76           12 S L73,L75

     FILE 'HCAOLD' ENTERED AT 10:10:31 ON 21 DEC 2003
L77            4 S L76

     FILE 'HCAPLUS' ENTERED AT 10:10:45 ON 21 DEC 2003
L78           30 S L76
L79           27 S L78 AND (PD<=20010208 OR PRD<=20010208 OR AD<=20010208)
L80            3 S L78 AND L47-L60
L81           29 S L63,L79-L80
L82            2 S L78 NOT L81

     FILE 'HCAOLD' ENTERED AT 10:12:46 ON 21 DEC 2003
                SEL AN L77
                EDIT /AN /OREF

     FILE 'HCAPLUS' ENTERED AT 10:13:12 ON 21 DEC 2003
L83            6 S E66-E69
L84            5 S L83 NOT MAZUR ?/AU
L85           31 S L81,L84
L86           26 S L81 NOT L84

     FILE 'REGISTRY' ENTERED AT 10:14:28 ON 21 DEC 2003

     FILE 'HCAOLD' ENTERED AT 10:14:44 ON 21 DEC 2003
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     FILE 'HCAPLUS' ENTERED AT 10:14:51 ON 21 DEC 2003
L87             3 S L84 AND L78
L88             5 S L84,L87
L89            22 S L86 NOT L63

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305813-59-6P 305813-60-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of cholestane compds. with a c17-alkyl side chain and an aromatic A-ring for use in cell modulating therapy)

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

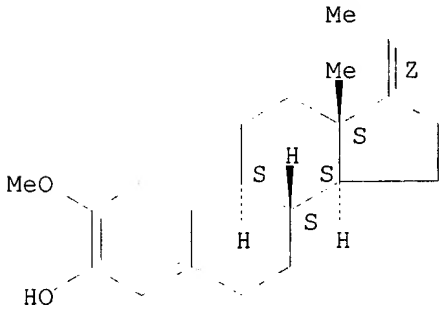
(1) Escaleira; 1993, 7, HCAPLUS
(2) Escaleira; J STEROID BIOCHEM MOL BIOL 1993, V45(4), P257 HCAPLUS
(3) Laing, S; US 3717627 A 1973
(4) Lajeunesse; 1994, 23, HCAPLUS
(5) Lajeunesse; BONE MINER 1994, V24(1), P1 HCAPLUS
(6) Liel; 1992, 25, HCAPLUS
(7) Liel; ENDOCRINOLOGY (BALTIMORE) 1992, V130(5), P2597 HCAPLUS
(8) Mountford; 1999, 8, HCAPLUS
(9) Mountford; EXP HEMATOL (N Y) 1999, V27(3), P451 HCAPLUS
(10) Ruggieri, P; US 3562260 A 1971 HCAPLUS

IT **229486-17-3P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of cholestane compds. with a c17-alkyl side chain and an aromatic A-ring for use in cell modulating therapy)

RN 229486-17-3 HCAPLUS
CN 19-Norpregna-1,3,5(10),17(20)-tetraen-3-ol, 2-methoxy-, (17Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

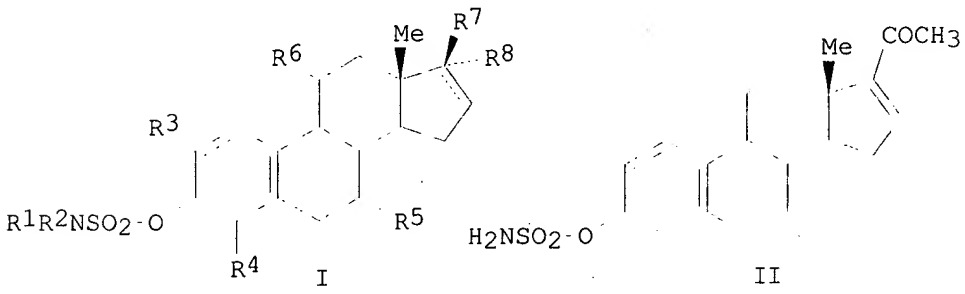


L41 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 1999:460438 HCAPLUS
DN 131:88083
ED Entered STN: 28 Jul 1999
TI Preparation of estrone sulfamate inhibitors of estrone sulfatase
IN Tanabe, Masato; Peters, Richard H.; Chao, Wan-Ru; Shigeno, Kazuhiko
PA SRI International, USA
SO PCT Int. Appl., 102 pp.
CODEN: PIXXD2

DT Patent
LA English
IC ICM C07J041-00
ICS A61K031-565; A61K031-57; A61K031-575
CC 32-3 (Steroids)
Section cross-reference(s): 2, 63
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9933858	A2	19990708	WO 1998-US27333	19981221
W: AU, CA, JP, KR				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 6046186	A	20000404	US 1997-997416	19971224
CA 2318349	AA	19990708	CA 1998-2318349	19981221
AU 9919416	A1	19990719	AU 1999-19416	19981221
AU 751732	B2	20020829		
EP 1042354	A2	20001011	EP 1998-964243	19981221
R: DE, FR, GB, IT, NL				
JP 2001527089	T2	20011225	JP 2000-526534	19981221
PRAI US 1997-997416	A	19971224		
WO 1998-US27333	W	19981221		

OS MARPAT 131:88083
GI



AB Novel compds.of formula I [R1, R2 = H, alkyl, etc.; R3 = H, CN, NO2, COOH, alkoxycarbonyl, etc.; R4 = H, NO2, (substituted) amino; R5, R6 = H, alkyl; R7, R8 = H, alkyl, alkenyl, alkynyl, alkoxy, acyl, acyloxy, etc.; R7,R8 = oxo, alkylidene, etc.] are prepared as inhibitors of estrone sulfatase. Thus, II is prepared from ethynylestradiol in 4 steps. and showed estrone sulfatase inhibitory activity of IC50 = 21 pM. Pharmaceutical compns. and methods for using I to treat estrogen-dependent disorders are provided.

ST estrone sulfamate prepn estrone sulfatase inhibitor
IT Estrogens
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(antiestrogens; preparation of estrone sulfamates as inhibitors of estrone sulfatase)
IT Antitumor agents
(preparation of estrone sulfamates as inhibitors of estrone sulfatase)
IT 59298-96-3, Estrone sulfatase
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(inhibitors; preparation of estrone sulfamates as inhibitors of estrone sulfatase)
IT 185910-34-3P 185910-42-3P 208924-86-1P 208924-87-2P 229485-78-3P

229485-79-4P 229485-80-7P 229485-81-8P 229485-82-9P 229485-83-0P
229485-84-1P 229485-85-2P 229485-86-3P 229485-87-4P 229485-88-5P
229485-89-6P 229485-90-9P 229485-91-0P 229485-92-1P 229485-93-2P
229485-94-3P 229485-95-4P 229485-96-5P 229485-97-6P 229485-98-7P
229485-99-8P 229486-00-4P 229486-01-5P 229486-02-6P 229486-03-7P
229486-04-8P 229486-05-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of estrone sulfamates as inhibitors of estrone sulfatase)

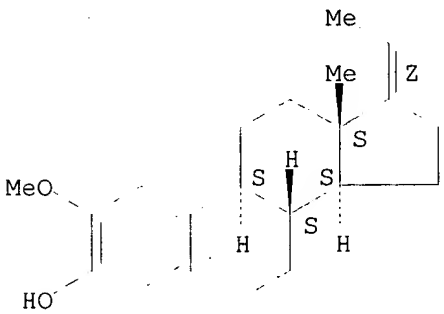
IT 50-28-2, Estradiol, reactions 53-16-7, Estrone, reactions 57-63-6, Ethynylestradiol 108-01-0, N,N-Dimethylethanolamine 109-77-3, Malononitrile 362-08-3 867-13-0, Triethylphosphonoacetate 1779-51-7, Butyltriphenylphosphonium bromide 4584-46-7 5407-04-5 6228-47-3, Propyltriphenylphosphonium bromide 7678-95-7 67530-18-1 229486-27-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of estrone sulfamates as inhibitors of estrone sulfatase)

IT 858-98-0P 1667-98-7P 4736-62-3P 5774-17-4P 5779-47-5P 5976-73-8P 5976-74-9P 6599-97-9P 13879-55-5P 13879-57-7P 14030-45-6P 14846-63-0P 14982-15-1P 15001-40-8P 22787-09-3P 23880-59-3P 31559-52-1P 57711-40-7P 59077-04-2P, 19-Norpregna-1,3,5(10)-trien-3-ol 59452-15-2P 59452-16-3P, 19,21-Dinorchola-1,3,5(10)-trien-3-ol 64215-82-3P 67519-62-4P 71716-18-2P 96111-26-1P 101766-63-6P 115208-23-6P 115387-92-3P 116627-15-7P 116627-20-4P 120574-27-8P 120574-28-9P 165619-18-1P 165619-19-2P 165619-20-5P 185910-40-1P 206442-55-9P 208758-44-5P 208758-45-6P 208758-46-7P 208758-49-0P 208758-50-3P 229486-06-0P 229486-07-1P 229486-08-2P 229486-09-3P 229486-10-6P 229486-11-7P 229486-12-8P 229486-13-9P 229486-14-0P 229486-15-1P 229486-16-2P **229486-17-3P** 229486-18-4P 229486-19-5P 229486-20-8P 229486-21-9P 229486-22-0P 229486-23-1P 229486-24-2P 229486-25-3P 229486-26-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of estrone sulfamates as inhibitors of estrone sulfatase)

IT **229486-17-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of estrone sulfamates as inhibitors of estrone sulfatase)

RN 229486-17-3 HCAPLUS
CN 19-Norpregna-1,3,5(10),17(20)-tetraen-3-ol, 2-methoxy-, (17Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L41 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 1998:397783 HCAPLUS
DN 129:54482
ED Entered STN: 29 Jun 1998

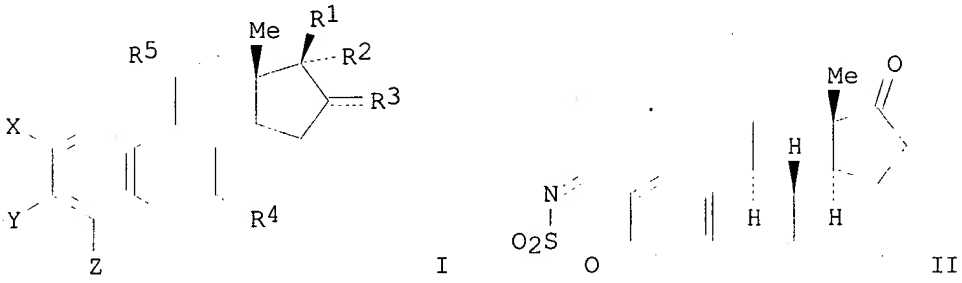
TI Preparation of steroid inhibitors of estrone sulfatase and associated pharmaceutical compositions and methods of use

IN Tanabe, Masato; Peters, Richard H.; Chao, Wan-ru; Shigeno, Kazuhiko
PA SRI International, USA

SO U.S., 23 pp.
CODEN: USXXAM
DT Patent
LA English
IC ICM A61K031-58
ICS C07J071-00
NCL 514176000
CC 32-3 (Steroids)
Section cross-reference(s): 1, 2
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 5763432	A	19980609	US 1997-794229	19970129
US 5861388	A	19990119	US 1997-1601	19971231
WO 9832763	A1	19980730	WO 1998-US1846	19980129

W: CA, JP, KR
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
PRAI US 1997-794229 19970129
OS MARPAT 129:54482
GI



AB Estratriene derivs. of formula I [X and Y, or Y and Z, form an oxathiazine dioxide ring or a dihydro-oxathiazine dioxide ring; R1, R2 = H, alkyl, alkynyl, (substituted) OH; R1R2 = O, S, (substituted) CH2; R3 = H, halo, alkyl, CH2; R4 = H, alkyl; R5 = H, OH, alkyl, alkenyl, alkoxy, aryl, CH2] are prepared as inhibitors of estrone sulfatase. Pharmaceutical compns. and methods for using I to treat estrogen-dependent disorders are provided as well. Thus, estradiol is transformed into II in 3 steps. In an estrone sulfatase inhibition assay, II showed 5-% inhibition at 9.3 nM.

ST estratriene deriv prepn estrone sulfatase inhibitor
IT 208758-20-7P 208758-22-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of steroid inhibitors of estrone sulfatase)
IT 208758-16-1P 208758-17-2P 208758-21-8P 208758-23-0P 208758-25-2P
208758-33-2P 208758-34-3P 208758-35-4P 208758-36-5P 208758-37-6P
208758-38-7P 208758-39-8P 208758-41-2P 208758-43-4P 208758-48-9P
208758-52-5P 208758-54-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of steroid inhibitors of estrone sulfatase)
IT 59298-96-3, Estrone sulfatase

RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(preparation of steroid inhibitors of estrone sulfatase)

IT 50-28-2, Estradiol, reactions 53-16-7, Estrone, reactions 57-63-6, 17α-Ethynylestradiol 1530-32-1, Ethyltriphenylphosphonium bromide 1779-51-7, Butyltriphenylphosphonium bromide 4954-12-5 6228-47-3, Propyltriphenylphosphonium bromide 7678-95-7 59077-04-2, 19-Norpregna-1,3,5(10)-trien-3-ol
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of steroid inhibitors of estrone sulfatase)

IT 4736-62-3P 6599-97-9P 13879-55-5P 13879-56-6P 31559-62-3P 34111-53-0P 57711-40-7P 64215-82-3P 99898-93-8P 120574-27-8P 120574-28-9P 123715-79-7P 137352-12-6P 206442-55-9P 208758-18-3P 208758-19-4P 208758-24-1P **208758-26-3P 208758-27-4P 208758-28-5P** 208758-29-6P 208758-30-9P 208758-31-0P 208758-32-1P 208758-40-1P 208758-42-3P 208758-44-5P 208758-45-6P 208758-46-7P **208758-47-8P** 208758-50-3P 208758-51-4P 208758-53-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of steroid inhibitors of estrone sulfatase)

IT 208758-49-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of steroid inhibitors of estrone sulfatase)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Babcock; US 4297350 1981 HCAPLUS

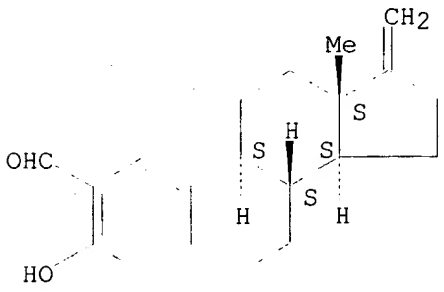
(2) Kuehne; US 3033860 1962 HCAPLUS

IT **208758-26-3P 208758-27-4P 208758-28-5P 208758-47-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of steroid inhibitors of estrone sulfatase)

RN 208758-26-3 HCAPLUS

CN Estra-1,3,5(10)-triene-2-carboxaldehyde, 3-hydroxy-17-methylene- (9CI) (CA INDEX NAME)

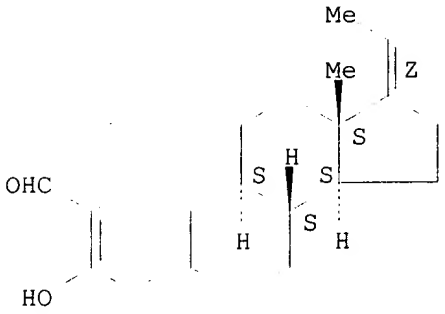
Absolute stereochemistry.



RN 208758-27-4 HCAPLUS

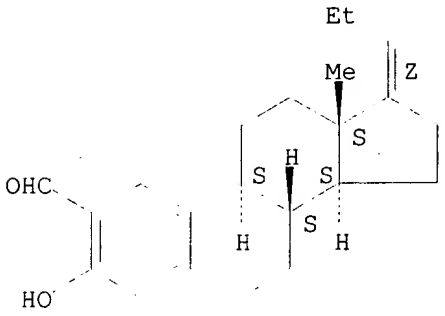
CN 19-Norpregna-1,3,5(10),17(20)-tetraene-2-carboxaldehyde, 3-hydroxy-, (17Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



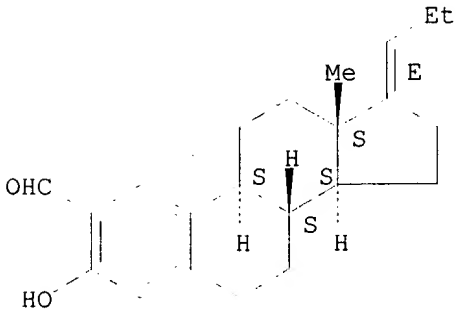
RN 208758-28-5 HCAPLUS
CN Estra-1,3,5(10)-triene-2-carboxaldehyde, 3-hydroxy-17-propylidene-, (17Z)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 208758-47-8 HCAPLUS
CN Estra-1,3,5(10)-triene-2-carboxaldehyde, 3-hydroxy-17-propylidene-, (17E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



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